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Collective Modes in an Inhomogeneous Electron Gas

Joyce Newman and Jerome K. Percus

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Computational Physics
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COLLECTIVE MODES IN AN INHOMOGENEOUS ELECTRON GAS

Joyce Newman and Jerome K. Percus

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ABSTRACT: This study is paralleled after J. Hubbard's treatment of collective modes in the uniform electron gas and differs mainly in the mathematical complexity. Large contributions to the correlation energy are identified with collective modes and this identification provides conditions for the frequency and lifetime of these modes. The contributions to the correlation energy are analyzed via diagramatic techniques where the Coulomb interaction between the electrons is replaced by a modified interaction. Only first order or "bubble" diagrams are considered and this is equivalent to the random phase approximation. The modified interaction is obtained from a certain integral equation whose solution is approximated by a variational principle. The kernel of this integral equation depends upon the density operator for the system of electrons with an external potential. The solution of the problem is formulated in two different ways, by using two different approximations for a closed form of the density operator. The first method uses a variational principle for the Green's function of the system and the second method uses a corrected Thomas-Fermi density operator which is valid for slowly varying potentials. Both methods require numerical techniques for their completion and these are carried out only for the second method. An application is made to atomic type systems and two undamped collective modes are found. One is a very singular resonance at 54Å and the other is a broad resonance between .24Å and .46Å.

CHAPTER I

Introduction

It is known that a free electron gas exhibits an undamped collective oscillation at the well established plasma frequency. We would like to study how an external potential affects the collective oscillation. In order for a collective mode to be well enough defined to be observed experimentally, it must not be heavily damped. This implies that, in particular, it is important to know how the inhomogeneity of the system affects the lifetime of the collective mode.

Several theoretical methods of studying the collective motions of a many body system exist. For example, in the theory of Tomonaga[1] a canonical transformation is made so that some of the new coordinates are directly related to the collective modes of motion and the remaining new coordinates are related to quasi-particle modes. In the theory of Bohm and Pines,[2] extra coordinates are introduced together with an equal number of subsidiary equations so that the correct number of degrees of freedom is preserved. A canonical transformation is then made so that the extra coordinates when transformed are related to the collective modes and the original coordinates when transformed are associated with quasi-particle modes. In both of these methods, the transformed Hamiltonian is separable with respect to the collective motion part. Though both of these methods are quite successful when studying the uniform electron gas, they are difficult to use for a system with an arbitrary external potential. First, it is not easy to generate the above mentioned canonical transformations for an arbitrary system. Second, in the Bohm and Pines theory it is difficult to find eigenfunctions which satisfy the subsidiary equations. Furthermore, with these methods, the interaction between the collective modes and the quasi-particle modes is not treated. This makes the damping problem difficult to study.

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[1] Tomonaga, S., Progr. Theor. Phys., Osaka 13 (1955) 467.

[2] Bohm, D. and Pines, D., Phys. Rev. 92 (1953) 609.

In a series of papers in 1957[3,4] Hubbard discusses a method which is applicable to an arbitrary fermion system in an external potential. His theory is based upon an infinite perturbation series which in principle is an exact solution of the many body problem and therefore contains all the physical effects including the collective motion. In his theory, the perturbation series is simplified by

---

[3] J. Hubbard, Proc. Royal Soc. (London) A240 (1957) 539-560.

[4] J. Hubbard, Proc. Royal Soc. (London) A244 (1958) 199-211.

replacing the interaction between the particles by a modified interaction. This modified interaction is equivalent to the modification of the ordinary interaction between the particles by the polarization of the medium represented by the remaining particles. Thus, Hubbard's theory is equivalent to a dielectric theory viewpoint where the electron gas is regarded as the dielectric medium. Using Hubbard's approach, the damping problem is easily treated. The specific calculations done in this paper are based upon these methods of Hubbard. Therefore, in the next section we present a detailed summary of Hubbard's many body perturbation theory.

CHAPTER II

Hubbard's Many Body Perturbation Theory[5]

1. Introduction

The problem is to determine the energy spectrum and wave functions of a gas of Fermi-Dirac particles which interact with one another through an instantaneous two-body potential v. It is assumed that the particles are moving so slowly that relativistic effects can be neglected.

The Hamiltonian for such a system is

$$H = H_0 + H'$$

where

$$H_0 = \sum_i \frac{p_i^2}{2m} + \sum_i U(\vec{x}_i) + \sum_i V(\vec{x}_i)$$

$$H' = \sum_{i \neq j} v(\vec{x}_i - \vec{x}_j) - \sum_i V(\vec{x}_i)$$

$\sum_i \frac{p_i^2}{2m}$ is the kinetic energy of the particles.

$U(\vec{x}_i)$ is the potential energy of each particle in an external field.

$\sum_{i \neq j} v(\vec{x}_i - \vec{x}_j)$ is the interaction energy of the particles.

and $V(\vec{x}_i)$ is introduced as a self-consistent field. The need for $V(\vec{x}_i)$ as well as a defining equation for for $V(\vec{x}_i)$ will be discussed in more detail in Section 7 of this chapter.

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[5] J. Hubbard, *Op. Cit.*

H' is treated as a perturbation.

2. The Perturbation Series.

The perturbation H' is assumed to be switched on adiabatically between $t = -\infty$ and $t = 0$ and adiabatically switched off between $t = 0$ and $t = \infty$. Then a system in an eigenstate ψ_0 of H_0 at $t = -\infty$ will slowly change into an eigenstate ψ of H. This result can be stated in the following form:

$$\psi = \lim_{\alpha \to +0} S_\alpha(0,-\infty)\psi_0 \;/\; (\psi_0|S_a(0,-\infty)|\psi_0)$$

is an eigenstate of H with the energy

$$E = E_0 + \Delta E = E_0 + \lim_{\alpha \to +0} (\psi_0|H' \; S_\alpha(0,-\infty)|\psi_0)/(\psi_0|S_\alpha(0,-\infty)|\psi_0$$

where E_0 is the energy of the unperturbed state ψ_0 and $S_\alpha(t,t')$ is the solution of the equation

$$(2.1) \quad i\hbar \frac{d}{dt} S_\alpha(t,t') = H_\alpha(t)\, S_\alpha(t,t')$$

with the boundary condition $S_\alpha(t',t') = 1$, where

$$(2.2) \quad H_\alpha(t) = e^{it/\hbar \, H_0} H' e^{-it/\hbar \, H_0} e^{-\alpha|t|} .$$

The limit $\alpha \to +0$ means $\alpha \to 0$ infinitely slowly. Equation (2.1) is equivalent to an integral equation

$$(2.3) \qquad S_\alpha(t) = 1 + \frac{1}{i\hbar}\int_{-\infty}^{t} H_\alpha(t')\, S_\alpha(t')\, dt'$$

where $S_\alpha(t)$ stands for $S_\alpha(t,-\infty)$.

The perturbation series is obtained by solving (2.2) by iteration.

$$(2.4) \quad S_\alpha(t) = 1 + \sum_{n=1}^{\infty} \left(\frac{1}{i\hbar}\right)^n \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \ldots \int_{-\infty}^{t_{n-1}} dt_n \; H_\alpha(t_1) H_\alpha(t_2) \ldots H_\alpha(t_n)$$

$$= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{1}{i\hbar}\right)^n \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 \ldots \int_{-\infty}^{t} dt_n \; P[H_\alpha(t_1) \ldots H_\alpha(t_n)]$$

(P is the chronological ordering operator which orders earliest times to the left.)

Using the notation of field theory, the perturbation H' is

$$(2.5) \quad H' = \frac{1}{2}\int [\bar\psi(\vec{x}\,')\psi(\vec{x}\,')v(\vec{x} - \vec{x}\,')\bar\psi(\vec{x})\psi(x)]\, d\vec{x}\, d\vec{x}\,'$$

$$- \frac{1}{2} N\, v(0) - \int \bar\psi(x)\; V(\vec{x})\; \psi(\vec{x})\, d\vec{x}$$

where $v(\vec{x}-\vec{x}\,')$ is the mutual potential energy of two particles at $\vec{x}$ and $\vec{x}\,'$ and N is the number of particles in the system. The second term subtracts the self-energies of the particles due to the interaction v since these are included in the first term. The last term represents the contribution from the self-consistent field. $\bar{\psi}(x)$ and $\psi(x)$ are the particle field operators and can be written in terms of an orthonormal basis $\{u_i\}$ as

$$\psi(x) = \sum_i u_i(\vec{x}) n_i$$

$$\bar{\psi}(x) = \sum_i \bar{u}_i(\vec{x}) \bar{n}_i$$

where $\bar{n}_i$ and n_i are creation and destruction operators for the particle in state i and since we have a fermion system $\bar{n}_i$ and n_i obey the anticommutation rules

$$0 = [n_i, n_j]_+ = [\bar{n}_i, \bar{n}_j]_+, \quad [n_i, \bar{n}_j]_+ = \delta_{ij} .$$

Here the $u_i(\vec{x})$ will be taken as eigenfunctions of the unperturbed one particle Hamiltonian,

$$(2.6) \quad [\frac{p^2}{2m} + U(\vec{x}) + V(\vec{x})] u_i(\vec{x}) = E_i u_i(\vec{x}) .$$

The second term of H', i.e. $-\frac{1}{2} N\, v(0)$, is a constant and will be included from now on in H_0 and not in H'.

If we write

x for $(\vec{x}, t)$

$v_\alpha(x-x')$ for $v(\vec{x} - \vec{x}')\delta(t-t')e^{-\alpha|t|}$

$\psi(x) = \psi(\vec{x}, t) = \sum_i u_i(x) n_i = \sum_i u_i(\vec{x}) e^{-i \frac{t}{\hbar} E_i} n_i$

$\bar{\psi}(x) = \sum_i \bar{u}_i(x) \bar{n}_i$

$V(x) = V(\vec{x}) e^{-\alpha|t|}$

and substitute equation (2.5) for H' into equation (2.2) for $H_\alpha(t)$, then equation (2.4) for $S_\alpha(t)$ becomes

$$(2.7) \quad S_\alpha(t) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\frac{1}{i\hbar}\right)^n$$

$$\times P\{[\tfrac{1}{2} \int dx_1 dx_1' (\bar\psi(x_1')\psi(x_1')v(x_1-x_1')\bar\psi(x_1)\psi(x_1)$$

$$- \int dx_1 \; \psi(x_1)V(x_1)\psi(x_1)] \times \ldots$$

$$\times [\tfrac{1}{2} \int dx_n dx_n' (\bar\psi(x_n')\psi(x_n')v(x_n-x_n')\bar\psi(x_n)\psi(x_n)$$

$$- \int dx_n \; \psi(x_n)V(x_n)\psi(x_n)]\}$$

where the integration is over all of space and for time from $t = -\infty$ to $t = t$.

3. Diagrammatic Interpretation of the Perturbation Series

It is convenient to re-express the particle field operators $\bar\psi(x)$ and $\psi(x)$ as

$$\psi(x) = \psi^+(x) + \psi^-(x), \quad \bar\psi(x) = \bar\psi^+(x) + \bar\psi^-(x)$$

where

$$\psi^-(x) = \sum_i^{unocc} u_i(x)n_i \quad \text{(destroys particles)}$$

$$\psi^+(x) = \sum_i^{occ} u_i(x)n_i \quad \text{(creates holes)}$$

$$\bar\psi^-(x) = \sum_i^{occ} \bar u_i(x)\bar n_i \quad \text{(destroys holes)}$$

$$\psi^+(x) = \sum_i^{unocc} \bar u_i(x)\bar n_i \quad \text{(creates particles).}$$

We are interested only in the operation of S_α on a particular eigenstate ψ_0 of H_0. It is assumed that ψ_0 is a non-degenerate eigenstate of H_0 in which certain definite states i are occupied. The state ψ_0 is then taken as the "redefined vacuum state".

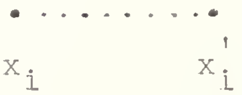
We then have

$$\psi^-(x)\psi_0 = 0 \tag{2.8}$$
$$\bar{\psi}^-(x)\psi_0 = 0 .$$

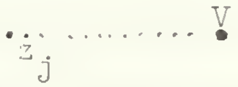
The P product in equation (2.7) is resolved in such a way as to move all the operators ψ^+, $\bar{\psi}^+$ to the left and all the operators ψ^-, $\bar{\psi}^-$ to the right, making use, of course, of the correct commutation rules. After this has been done, because of equations (2.8), all the terms involving ψ^- and $\bar{\psi}^-$ can be omitted.

It is then found that the remaining terms contributing to $S_\alpha(t)\psi_0$ can be conveniently classified according to diagrams similar to Feynmann diagrams. There is a one to one correspondence between each diagram and each term contributing to $S_\alpha(t)$. We now give the prescriptions for drawing these diagrams and then for calculating the corresponding contribution to $S_\alpha(t)$.

1. Mark p points on the diagram and label them $x_1, x_2, \ldots, x_p$. Mark another set of p points and label them with $x_1', x_2', \ldots, x_p'$. Join the pairs of points x_i, x_i' by interaction lines (usually signified by broken lines)



2. Mark m points $z_1, z_2, \ldots, z_m$ and from each of these draw a V line (usually signified by a broken line to a small filled in circle marked V).



3. Draw directed particle lines, one entering and one leaving each of the points x_i, x_i', z_j. These lines may run between points, from a point to itself, or from a point to the edge of the diagram or from the edge of the diagram to the point.

The order n of a diagram equals the sum of the interaction lines plus the V lines, i.e.

$$n = p + m .$$

The different n-th order diagrams are obtained by drawing in the particle lines in all possible ways.

The contribution to $S_\alpha(t)$ corresponding to a given diagram is:

1. For every interaction line $x_i \; x_i'$ introduce a factor $\frac{1}{2i\hbar} \, v(x_i - x_i')$ and an integration with respect to $dx_i \; dx_i'$ over the region of space time behind the surface t.
2. For every V line whose vertex is labelled x_j introduce into the integrand a factor $-\frac{1}{i\hbar} \, V(x_j)$ and an integration over dx_j.
3. For every particle line from a point y ($= x_i, x_i'$ or z_j) to the edge of the diagram introduce a factor $\bar{\psi}^+(y)$ into the integrand. For every particle line from the edge of the paper to a point y introduce $\psi^+(y)$ into the integrand. If $\psi^+(y)$ corresponds to an incoming line and $\bar{\psi}^+(z)$ to the corresponding outgoing line, then $\bar{\psi}^+(z)$ is adjacent to and on the left of $\psi^+(y)$.
4. For every particle line from a point y to a point z ($z \neq y$) introduce a factor $S(z,y)$ into the integrand.
5. For every particle line running from a point y to itself introduce a factor $\rho(y)$ into the integrand.
6. Multiply the integral by $\frac{1}{n!} \, (-1)^q$ where n is the order of the diagram and q is the number of closed particle loops.

The quantity $\rho(x)$ is the charge density corresponding to ψ_0, i.e.

$$\rho(x) = \sum_i^{occ} \bar{u}(\vec{x}) \; u_i(\vec{x}) \; .$$

The $u_i(\vec{x})$ were defined in equation (II.6).

$$u_i(x) = u_i(\vec{x})\, e^{-\frac{it}{\hbar} E_i} .$$

$S(x',x)$ is a propagator which is a solution of:

$$[i\hbar \frac{\partial}{\partial t'} + \frac{\hbar^2}{2m} \nabla'^2 - u(\vec{x}')]\, S(x',x) = \delta(\vec{x}-\vec{x}')\delta(t-t')$$

and

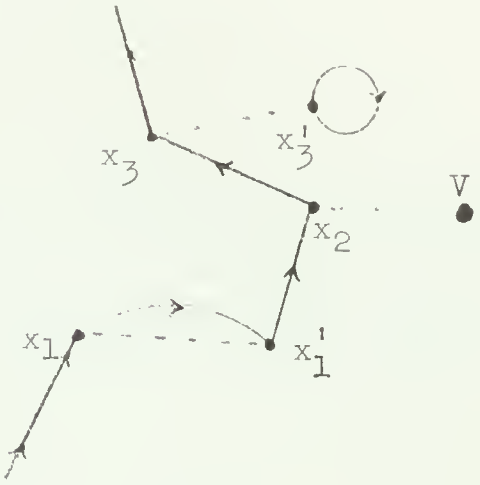
$$(2.9) \qquad S(x',x) = \theta(t'-t) \sum_i^{\text{unocc}} u_i(x')\, \bar{u}_i(x) - \theta(t-t') \sum_i^{\text{occ}} u_i(x')\, \bar{u}_i(x)$$

$$\theta(t) = 1 \quad \text{if } t > 0$$
$$= 0 \qquad t < 0$$
$$= \tfrac{1}{2} \qquad t = 0 .$$

Note that when $t = t'$, $S(x,x')$ reduces to $\frac{1}{2} - \rho(\vec{x},\vec{x}')$ where $\rho(\vec{x},\vec{x}')$ is the Dirac density matrix corresponding to the state ψ_0, i.e.

$$\rho(\vec{x},\vec{x}') = \sum_i^{\text{occ}} u_i(\vec{x})\, \bar{u}_i(\vec{x}') .$$

To clarify the above prescriptions consider the following diagram:



The contribution of this diagram to $S_\alpha(t)$ is

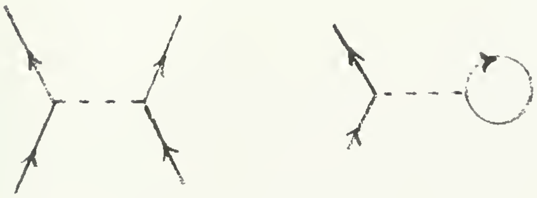
$$\frac{+1}{3!}\left(\frac{1}{2i\hbar}\right)^2\left(\frac{-1}{i\hbar}\right) \int dx_1 dx' dx_2 dx_3 dx_3' [v_\alpha(x_1-x_1')v_\alpha(x_3-x_3')V_\alpha(\vec{x}_2)$$

$$\cdot\ \bar{\psi}^+(x_1)\psi^+(x_3)\ S\ (x_1',x_1)\ S(x_2,x_1')\ S(x_3,x_2)\rho(x_3')].$$

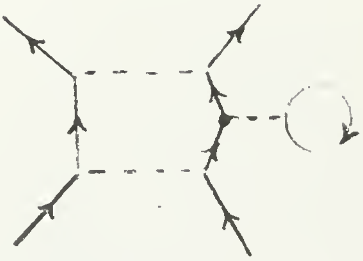
4. The Linked Cluster Expansion.

The perturbation series for the energy as derived above contains terms which diverge more strongly than N, the number of particles in the system, as N –> ∞. Such terms can have no physical significance and it should be possible to eliminate them from the series. This is the basis for the linked-cluster expansion.

A diagram may fall into two or more unconnected parts. Such a diagram is described as unlinked. Otherwise it is called linked. For example:



unlinked



linked

It is the unlinked diagrams which have no physical significance and which can be eliminated from consideration.

It can be shown that

$$S_\alpha(t) = \exp\{S_{L_\alpha}(t)\}$$

where

$$S_{L_\alpha}(t) = \sum_{\Gamma}^{\text{linked}} S_\alpha(t,\Gamma)$$

The sum is over all linked structures Γ. Note that it is structures which are summed and not diagrams. Diagrams which have the same arrangement of vertices, interaction, V, and particle lines and differ only in the labeling of vertices are said to have the same structure.

$S_{L_\alpha}(t)$ can be resolved into two parts:

$$S_{L_\alpha}(t) = S_{L_\alpha}^{(0)}(t) + S_{L_\alpha}^{'}(t) .$$

$S_{L_\alpha}^{(0)}(t)$ contains the contributions from all linked vacuum diagrams i.e. diagrams without particle lines going to or from the edge of the diagram. Hence $S_{L_\alpha}^{(0)}(t)$ contains no operators and is a c number.

$S_{L_\alpha}^{'}(t)$ contains the contributions of all linked diagrams with external lines.

It follows that:

1. $$\psi = c \lim_{\alpha \to +0} \exp\,(S_{L_\alpha}^{'}(0))\psi_0,$$

c is a normalization factor.

2. whereas ΔE requires only a vacuum expectation:

Write down the sum of all integrals contributing to $S^{(0)}_{L_\alpha}(\infty)$ (one from each vacuum diagram). Put a factor $i\hbar\,\delta(t_1)$ into each of these integrands and put $\alpha = 0$. The resulting sum gives ΔE.

5. Polarization Parts and the Modified Interaction.

Consider the following subdiagram:

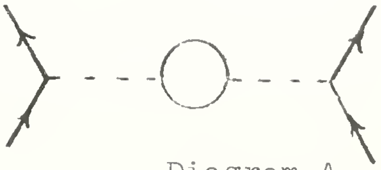
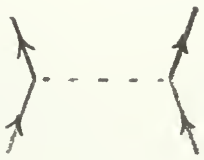


Diagram A

The circle represents some set of closed particle loops and interaction lines which are connected to the rest of the diagram by only two interaction lines as shown in the diagram. This subdiagram represents the scattering of two particles through some complicated process which, however, returns the particles involved to their original states. Hubbard shows that subdiagrams of this sort represent the polarization effect and can be eliminated from the perturbation series by replacing the ordinary interaction by a modified interaction.

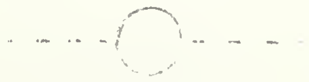
The term polarization part is used to describe some connected part without external lines which is connected to the rest of the diagram by only two interaction lines. For example, the circle in the above diagram is a polarization part.

Suppose Γ is some structure. If Γ contains one or more polarization parts Γ is called (polarization) reducible. Otherwise, Γ is irreducible. All reducible structures can be obtained by inserting polarization parts in place of interaction lines in irreducible structures. For example, the above diagram A can be obtained from the following irreducible one, B, by replacing the interaction line with the polarization part C.



irreducible

Diagram B



polarization part

Diagram C

Furthermore, all reducible structures are uniquely reducible i.e., any reducible structure arises from a unique irreducible one.

Consider a given irreducible structure Γ'. Then it can be shown that the total contribution to $S'_L(t)$ of all diagrams with structures which reduce to Γ' is:

$$S(t,\Gamma';V_t)$$

where this expression means the contribution to $S(t)$ from a diagram with structure Γ' and with all interactions v replaced everywhere by V_t, and

$$(2.10) \qquad V_t(x',x) \equiv \sum_{\substack{\text{all possible}\\ \text{polarization}\\ \text{parts}}} W_t(x',x,\Gamma_s')$$

where $W_t(x',x,\Gamma_s')$ is the contribution from a polarization part Γ_s'.

Therefore the total $S_L(t)$ is a sum over all irreducible diagrams with v replaced by V_t in all the integrals. Thus V_t plays the part of a modified interaction.

For calculating the wave function V_0 (i.e. V at time equals zero) is needed; for the energy shift ΔE, V_∞ (time at infinity) is needed.

For a correct counting of diagrams one gets the following expression for the total energy shift ΔE:

$$(2.11) \qquad \Delta E = \overset{\substack{\text{irreducible}\\ \text{vacuum}}}{\sum_{G}} \int_0^\lambda \frac{d\lambda}{\lambda}\, n(G)\, \Delta E_v(G) \;;$$

$n(G)$ is the order of the diagram G.

The interaction v is regarded as being linearly proportional to some coupling constant λ.

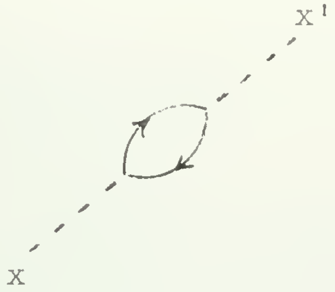
$\Delta E_v(G)$ means the contribution of the diagram G to ΔE with v replaced everywhere by V_∞. (Henceforth V_∞ will be designated as V.)

The sum is over all irreducible vacuum diagrams.

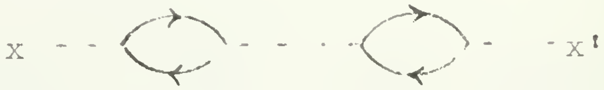
6. An Integral Equation for the Modified Interaction.

The modified interaction V has been defined as an infinite sum over all polarization parts. This is not a rapidly convergent series. It will now be shown that there exists an integral equation for V and that this allows us to calculate V from a series which is rapidly convergent.

A polarization structure which consists of two or more parts which are connected only by single interaction lines is called an improper polarization part. If the structure cannot be resolved into at least two parts which are connected by a single interaction line, it is called a proper polarization part. For example, diagram D is a proper polarization part and diagram E is an improper one.



D



E

Suppose Γ is some improper polarization part. Then it can be uniquely resolved into a proper part and some other polarization part, proper or improper.

Let $W(x',x,\Gamma)$ stand for the contribution to $S_\alpha(t)$ from the diagram Γ. Define $\overline{W}(x',x\ \Gamma)$ by:

(2.12) $W(x',x,\Gamma) = \int v(x'-x'')\, \overline{W}(x'',x''',\Gamma)\, v(x'''-x)\, dx''\, dx'''$

The two v's correspond to the two outgoing interaction lines of the polarization structure and $\overline{W}$ corresponds to the rest of the structure. See diagram F as an example.

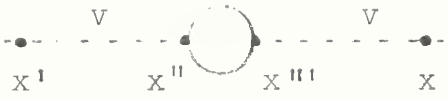


Diagram F

The whole diagram contributes W and the part within the circle contributes $\overline{W}$. For the example shown in diagram D, $\overline{W}$ is

(2.13) $$\overline{W} = -\frac{1}{i\hbar} S(x',x)\, S(x,x')$$

If the improper structure Γ is resolved into a proper part Γ' and another part Γ'',

(2.14) $$W(x',x,\Gamma) = \int v(x'-x_1)\, \overline{W}(x_1,x_2,\Gamma')\, v(x_2-x_3) \cdot \overline{W}(x_3,x_4,\Gamma'')\, v(x_4-x)\, dx_1\, dx_2\, dx_3\, dx_4 .$$

Define $W^*(x',x,\Gamma')$ as

(2.15) $$W^*(x',x,\Gamma') = \int v(x'-x'')\, \overline{W}(x'',x,\Gamma')\, dx''$$

and (2.14) becomes

(2.16) $$W(x',x,\Gamma) = \int W^*(x',x'',\Gamma')\, W(x'',x,\Gamma'')\, dx'' .$$

The total contribution to V from all improper structures which resolve into the proper part Γ' is obtained by summing over all structures Γ''. From the right side of (2.16) this sum is

$$(2.17)\quad \int W^{*}(x',x'',\Gamma') \sum_{\Gamma''} (x'',x,\Gamma'')\,dx''$$

$$= \int W^{*}(x',x'',\Gamma') \left[v(x''-x') + \sum_{\Gamma''\neq\Gamma_0} W(x'',x,\Gamma'')\right] dx''$$

where $v(x''-x')$ is equivalent to Γ_0. But the sum over all polarization structures Γ'' is just the definition of V. Thus (2.17) can be written as

$$(2.18)\qquad \int W^{*}(x',x'',\Gamma')\, V(x'',x)\, dx'' .$$

This is the contribution to V of the proper part Γ' and all the improper parts which resolve into Γ'. To obtain the total V, (2.18) must be summed over all proper polarization parts Γ'.

Let

$$(2.19)\qquad V^{*}(x',x) = \sum_{\Gamma'\neq\Gamma_0}^{\text{proper}} W^{*}(x',x,\Gamma')$$

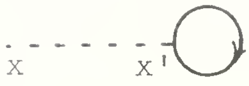
so

$$(2.20)\quad V(x',x) = v(x'-x) + \int V^{*}(x',x'')\, V(x'',x)\, dx'' .$$

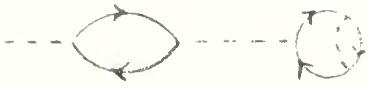
7. The Self-Consistent Field.

The remarks in this section apply only to vacuum diagrams (those without external lines). As has been discussed previously, these are the only diagrams which contribute to the energy shift.

Any part of a diagram which is connected to the rest of the diagram by only a single interaction line is called an H-part. For example, diagrams G and H are both H parts.



G



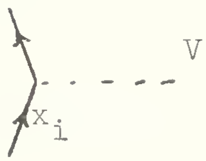
H

If there is no external potential then it can be shown that diagrams containing H parts do not contribute to the energy. The proof depends upon the uniformity of the gas and so does not apply when there is an external potential. However, the potential V can be chosen in such a way so that the H parts can be eliminated.

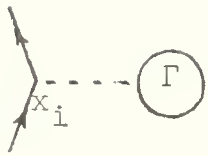
If the H part can be resolved into a polarization part and, some other H part, it is called improper. Otherwise it is proper. For example diagram G is proper and diagram H is improper.

An H part Γ gives a factor which we will denote by $H(x_i,\Gamma)$. There is no preferred origin of time in the theory so that $H(x_i,\Gamma)$ is independent of time, and can be written as $H(\vec{x}_i,\Gamma)$.

We can choose V(x) so that the subdiagram I cancels the sum of all subdiagrams J. (In diagram J, Γ is a proper H part.)



I



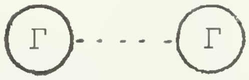
J

If a correct counting of diagrams is performed, it can be shown that the choice for V(x) is

$$V(\vec{x}) = \sum_{\Gamma} \frac{2^{n(\Gamma)}}{g(\Gamma)} H'(\vec{x},\Gamma) \quad . \tag{2.21}$$

The sum is over all proper H parts; $n(\Gamma)$ is the order of the H part Γ, $g(\Gamma)$ is the number of permutations of the interaction lines which leave Γ unchanged.

With this choice for V one can eliminate all diagrams containing H parts with the exception of symmetrical diagrams of the type shown in diagram K.



K

The total contribution to the energy from these types of diagrams can be shown to be

$$(2.22) \quad E_H = - \sum_{\Gamma} \frac{2^{2n(\Gamma)-1}}{[g(\Gamma)]^2} \int H(\vec{x},\Gamma)\, v(x-x')\, H(x',\Gamma)\, d\vec{x}\, d\vec{x}'.$$

The simplest H part is that shown in diagram G. If all other H parts are neglected, we have

$$(2.23) \qquad V(\vec{x}) = \int v(\vec{x}-\vec{x}')\, \rho(\vec{x}')\, dx'$$

which is the same as the symmetrized Hartree field. Therefore, the self-consistent field introduced in this section is a generalization of the ordinary Hartree field. Keeping only the simplest H part,

$$(2.24) \qquad E_H = - \frac{1}{2} \int \rho(\vec{x})\, v(\vec{x}-x')\, \rho(x')\, d\vec{x}\, d\vec{x}' ,$$

which is the term which must be subtracted when calculating the total energy in an ordinary Hartree calculation.

The calculation of $V(\vec{x})$ from (2.21) is a self-consistent calculation since $H'(\vec{x},\Gamma)$ depends upon the density $\rho(\vec{x})$ and the propagator $S(x',x)$. These depend upon the $u_i(\vec{x})$ and E_i which in turn depend upon $V(\vec{x})$. (See equation (2.6).)

8. The Energy Shift and Collective Modes.

Making use of equation (2.11) and of correct counting procedures, it can be shown that the energy shift ΔE is

$$(2.25)\quad \Delta E = \frac{i\hbar}{2}\int_0^\lambda \frac{d\lambda}{\lambda}\int dx_1 \int dx_1' \, \delta(t_1)\, \overline{V}(x_1,x_1')V(x_1',x_1)$$

$$(2.26)\quad \overline{V}(x',x) = \sum_{\Gamma\neq\Gamma_0}^{\text{proper}} \overline{W}(x',x\ \Gamma)$$

where $\overline{W}$ has been defined in equation (2.12) and the definition of proper is discussed just prior to equation (2.12).

From equations (2.15) and (2.19) we have

$$(2.27)\quad V^*(x',x) = \int \overline{V}(x',x'')\ v(x''-x)\ dx$$

and (2.20) can be used to calculate $V(x',x_1)$

$$(2.20)\quad V(x_1',x_1) = v(x_1'-x_1) + \int V^*(x_1',x'')\ V(x'',x_1)\ dx'' \ .$$

The total energy of the system is

$$(2.28)\quad E = \sum_i^{\text{occ}} E_i - \frac{1}{2}Nv(0) + E_H + \frac{i\hbar}{2}\int_0^\lambda \frac{d\lambda}{\lambda}\int dx\ dx'$$

$$\cdot\ \delta(t)\ V(x,x')\ \overline{V}(x',x)\ .$$

In order to study ΔE we must solve the integral equation (2.20). For a uniform gas, this solution is easily done by Fourier transformation. For the non-uniform case we need a different method which will now be described.

Multiply equation (2.28) by $\bar{V}(x,x'')$ and integrate over x''. Then

$$(2.29) \quad F(x',x) = V^*(x',x) + \int V^*(x',x'')\, F(x'',x)\, dx''$$

where

$$(2.30) \quad F(x',x) = \int V(x',x'')\, \bar{V}(x'',x)\, dx''$$

$$(2.27) \quad V^*(x',x) = \int \bar{V}(x',x'')\, v(x''-x)\, dx''$$

$$(2.30) \quad \Delta E = \frac{i\hbar}{2} \int_0^{\lambda} \frac{d\lambda}{\lambda} \int dx\; \delta(t)\, F(x,x) \; .$$

It is still possible to Fourier transform with respect to the time difference.

$$(2.31) \quad F(\vec{x}',\vec{x},\omega') = V^*(\vec{x}',\vec{x}\;\omega') + \int V^*(\vec{x}',\vec{x}'',\omega')F(\vec{x}'',\vec{x}\;\omega')d\vec{x}''$$

$$(2.32) \quad \Delta E = \frac{i\hbar}{4\pi} \int_0^{\lambda} \frac{d\lambda}{\lambda} \int d\omega'\; d\vec{x}\; F(\vec{x},\vec{x},\omega')$$

To solve equation (2.29), introduce the eigenvalues and eigenfunctions of the homogeneous equations

$$(2.33) \quad \begin{aligned} \mu_i(\omega')\phi_i(\vec{x},\omega') &= \int V^*(\vec{x},\vec{x}',\omega')\phi_i(\vec{x}',\omega')\; dx' \\ \mu_i(\omega')\chi(\vec{x},\omega') &= \int V^*(\vec{x}',\vec{x},\omega')\chi_i(\vec{x}',\omega')\; dx' \; . \end{aligned}$$

If $F(\vec{x}',\vec{x},\omega')$ is expanded in terms of the $\Phi_i(x')$ and $\psi_j(x)$[6] and use is made of the orthonormality relations between the $\psi_j(x)$ and $\Phi_i(x)$, we can solve equation (2.31) and equation (2.32) reduces to

$$(2.34) \qquad \Delta E = \frac{i\hbar}{4\pi} \int_0^\lambda \frac{d\lambda}{\lambda} \int d\omega' \frac{\sum_i h_i(\omega')\, \mu_i(\omega')}{1 - \mu_i(\omega')}$$

where $h_i(\omega')$ is the degeneracy of the eigenvalue $\mu_i(\omega')$. Writing $\mu_i(\omega') = A_i(\omega') + i\, \Sigma_i(\omega')$ and remembering that ΔE must be real

$$(2.35) \qquad \Delta E = -\frac{\hbar}{4\pi} \int_0^\lambda \frac{d\lambda}{\lambda} \int d\omega' \frac{\sum_i h_i(\omega')\, \Sigma_i(\omega')}{[1-A_i(\omega')]^2 + \Sigma_i^2(\omega')}$$

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[6] Since $V^*(\vec{x}',\vec{x}'',\omega')$ is not necessarily a self-adjoint operator, we realize that the solutions Φ_i and χ_i of the homogeneous equations may not form a complete set. However, we note that any operator can be put into Jordan canonical form and also that (2.31) can be written as $F = (1-V^*)^{-1}V^*$. In (2.32) we are interested in Tr F. Using these facts we can show that the lack of a complete set simply causes a modification of the weighting factor $h(\omega')$ in (2.34).

There will be a large contribution to the energy at those frequencies ω' for which any $A_i(\omega') = 1$ provided $\Sigma(\omega')$ is small. These large contributions to the energy can be associated with collective modes. The frequency of these modes is given by $A_i(\omega') = 1$ and $\Sigma(\omega')$ describes the damping. If $\Sigma(\omega')$ is large it will not be possible to recognize the collective modes. Thus the conditions for a collective mode are

$$\begin{aligned} A_i(\omega') &= 1 \\ \Sigma_i(\omega') &= 0 \,. \end{aligned} \tag{2.36}$$

We will show more explicitly in the next chapter that equations (2.36) really do correspond to a collective state. Also, in Chapter IV we will see that these equations lead to an accurate prediction of the collective modes for a free gas.

CHAPTER III

Physical Interpretation of the Collective Mode[7]

1. General Remarks.

Experimentally, one measures the excitations of a many body system by means of an external probe such as inelastically scattered particles or X-rays. For example, the experiment might measure the energy distribution or the angular distribution of the scattering cross-section.

If the density of the many body system is $\rho(r)$ we can write

$$\rho(r) = \sum_i \delta(r-r_i) = \sum_k \rho_k e^{ik\cdot r} = \sum_{i\,k} e^{i k\cdot(r-r_i)}$$

where ρ_k is called the density fluctuation and is defined as

$$\rho_k = \sum_i e^{i k\cdot r_i}$$

This ρ_k describes the fluctuations in particle density about the average density. The probability that the external probe transfer momentum k and energy ω to the many body system is proportional to

$$\sum_n (\rho_k^+)^2_{n0} \delta(\omega-\omega_{n0})$$

where the ω_{n0} are the exact excitation frequencies of the many body system induced by the density fluctuations ρ_k^+. The proportionality factor depends only on the interaction v(r) between the incoming probe and the target particle and not on any dynamical properties of the many body system. For example, if the Born approximation applies, this factor would be $2\pi v_k^2$ where

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[7] General references for this chapter are:
D. Pines, The Many Body Problem, pp. 1-69, New York (1962).
D. Pines, Elementary Excitations in Solids, pp. 56-165 New York, (1964).

$$v_k = \int v(r)\, e^{ik\cdot r}\, d^3r \; .$$

The maximum experimental information about the many body system is therefore contained in the quantity

$$S(k\omega) = \sum_n |\rho_k^+|_{n0}^2 \, \delta(\omega-\omega_{n0}) \; .$$

$S(k\omega)$ is the Fourier transform in space and time of the time dependent pair-distribution function for the many body system. It is the spectrum of excitations available to the density fluctuations ρ_k that is actually measured, i.e. the excited states are coupled to the ground state by the density fluctuation ρ_k.

For a non-interacting fermion system, the density fluctuation spectrum coincides with simple single particle-hole pairs.

Consider now a fermion system with an interacting potential between all the particles. This interaction causes correlations in particle positions and these correlations cause coherence effects. In a dense electron gas, the correlations give rise to screening i.e. each electron polarizes its immediate surroundings. The density fluctuation excitation spectrum will contain instead of simple particle hole pairs, quasi-particle hole pairs. The quasi-particle is the particle plus a screening cloud. In addition, sometimes it is possible that the correlations give rise to coherence factors which greatly reduce the probability for exciting single quasi-particle pairs. Instead, there may be a coherent superposition of particle hole pairs which is referred to as a collective mode. The collective state differs from the quasi-particle states both in amplitude and spacing. The amplitude of a collective state is proportional to N, the number of particles in the system. Single particle amplitudes are not proportional to N. Also, for a given momentum transfer we would expect collective states to be widely spaced whereas single particle states are close together. Also, since it is a coherence of density fluctuation excitations, the collective mode corresponds to oscillations in the particle density. For this reason, when speaking of free gases, collective modes are sometimes referred to in the literature as zero sound. However, unlike sound waves it is not the frequent collision of particles which acts as the restoring force. The restoring force is the averaged force field of a large number of interacting particles. Collisions between the particles in a gas would disrupt this averaged field and damp the collective mode. Therefore, we would expect collective modes to be observed only if $\omega\tau >> 1$, where τ is the average time between collisions. This condition is satisfied at low temperatures. In this paper, we assume the temperature to be zero, so the above condition is always satisfied. This assumption is valid for a system such as an atom at room temperature. However, in a stellar system where the temperature is very high the results of this paper would not be valid. Furthermore, we might expect that in a star we would not observe any collective modes as they might be heavily damped due to particle collisions.

For collective modes to exist and to be observable there is another requirement. They must not decay quickly into single quasi-particle pairs. Either this decay must not be energetically possible or else, because of coherence effects between the relevant matrix elements, the probability for exciting these single particle-hole pairs must be greatly reduced. If this probability is high, the collective mode would be very quickly damped and so unobservable. If this probability is zero, then the collective mode can be a long lived well defined excitation of the system. The damping term referred to in this paper is a measure of this probability for exciting single quasi-particle hole pairs.

2. Relation to the Dielectric Constant.

The Fourier transforms in time of the macroscopic Poisson equations are:

$$\operatorname{div} D(\omega) = \varepsilon(\omega) \operatorname{div} E(\omega) = 4\pi q(\omega)$$

$$\operatorname{div} E(\omega) = 4\pi [q(\omega) - e\langle\rho(\omega)\rangle]$$

where $q(\omega)$ is the true free charge and $e\langle\rho(\omega)\rangle$ represents the polarization charge. If $q(\omega)$ represents an external probe, then $\rho(\omega)$ represents the response of the system. A collective mode corresponds to a free resonance in the system, i.e., in the absence of any external q there must be a fluctuating non-zero electric field $E(\omega)$ and also a non-zero fluctuation in $\langle\rho(\omega)\rangle$. The only way for E and ρ to be nonzero if q is zero is for some eigenvalue of the dielectric constant operator to be zero. So a collective mode corresponds to the condition that $\varepsilon(\omega)$ is singular.

It has been shown by Nozières and Pines[8] that the shift in the total energy of the system due to the interaction between the electrons can be written in the form:

$$(3.1) \quad E_{\text{int}} = - \int_0^\infty \frac{d\omega}{2\pi} \operatorname{Im} \operatorname{Tr} \left[\varepsilon(\omega)^{-1} + \frac{Ne^2}{r}\right] ,$$

where by Im we mean the skew hermitian part.

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[8] P. Nozières and D. Pines, Il Nuovo Cimento [x], 9, (1958), pp. 470-489.

Actually Nozières and Pines derived this relationship for a uniform system where $\varepsilon(\omega)$ is diagonal in a plane wave representation. We believe their proof can be generalized so that a relation very similar to (3.1) is true for a non-uniform system.

We must subtract the term Ne^2/r so that this definition of the energy shift coincides with the energy shift defined in equation (2.25). From equation (2.34) we have

$$(2.34) \quad \Delta E = \mathrm{Re}\, \Big[\frac{i\hbar}{4\pi} \sum_i \int_0^{\lambda} \frac{d\lambda}{\lambda} \int d\omega' \, \frac{h_i(\omega')\mu_i(\omega')}{1 - \mu_i(\omega')}$$

where $h(\omega\ )$ is the degeneracy of each $\mu(\omega')$.

It is not hard to show from (3.1) that

$$(3.2) \quad \Delta E = - \int_0^{\lambda} \frac{d\lambda}{\lambda} \int \frac{d\omega}{2\pi} \, \mathrm{Im}\, \Big[\mathrm{Tr}\, \Big[\frac{1}{\varepsilon(\omega)} \Big] \Big] \, .$$

By comparing these two equations, we see that the condition for a collective mode that was previously stated, i.e. that $\mu(\omega') = 1$, is completely equivalent to the condition that $\varepsilon(\omega)$ be singular.

We think that a collective state in a non-uniform system is a new type of excitation and as such would not show up by perturbational treatment. This means on the one hand that if the non-uniformity is treated perturbationally with respect to the free gas the result will be the same as in the free gas. We show this in Appendix C. On the other hand, Atlick and Glassgold[9] have shown that the correlation energies for single particle states when calculated in the random phase approximation are quite small corrections to the Hartree-Fock energies. Therefore, we think that a very large contribution to the correlation energy must correspond to a new type of excitation, namely a collective state.

3. Structure Factor S(k) and the Spectral Function S(k,ω)

Pines has derived a useful relationship[10]

$$\operatorname{Im} \frac{1}{\varepsilon(k\omega)} = - \frac{4\pi^2 e^2}{k^2} S(k\omega) , \qquad \omega > 0 .$$

Thus a zero in $\varepsilon(k\omega)$ should correspond to a peak in $S(k\omega)$. ($S(k\omega)$ has already been defined.)

The structure factor, $S(k)$, $= \langle \psi_0 | \rho_k^+ \rho_k | \psi_0 \rangle / N$ and is the Fourier transform of the time-independent pair distribution function.

$S(\vec{k})$ is related to $S(\vec{k}\omega)$ by

$$\int_{-\infty}^{\infty} d\omega \, S(\vec{k}\omega) = S(\vec{k})N .$$

If we refer back to the introduction we see that there may be more than one discrete eigenvalue $\mu_i(\omega)$. Each of these eigenvalues may yield one or more (or perhaps none) collective modes. If we knew the complete solution, i.e. all the collective modes and all the eigenvalues we would have the equivalent of a discrete dispersion relation. In the free gas case the index i becomes equivalent to the continuous wave vector $\vec{k}$, and $\mu_i(\omega)$ is replaced by $\mu(k\omega)$. The collective mode condition $1- (\vec{k}\omega) = 0$ provides a dispersion relation $\omega(k)$. We do not have such complete information here as we have evaluated only one eigenvalue. We know at what frequency ω_0 to expect a collective resonance but we do not have a dispersion relation. Therefore, we know that $S(\vec{k}\omega)$ has a peak at ω_0 but we do not know the complete form for $S(k\omega)$ and so we cannot evaluate $S(k)$. These remarks can be illustrated more clearly. R. D. Puff [15] has shown that for a single resonance $\omega_0(k)$ with zero damping

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[9] Atlick and Glassgold, Phys. Rev. 133 (1964) A632-A646.

[10] D. Pines, The Many Body Problem, p. 38, N. Y. (1962).

$$S(k\omega) = \frac{2\pi N\ k^2/2m}{\omega_0(k)} \left(\delta(\omega-\omega_0(k)) + \delta(\omega + \omega_0(k)\right) .$$

There is a sum rule

$$\frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \coth \frac{1}{2}\, \beta\omega\left(\frac{2m}{k^2}\right) S(k\omega) = \frac{S(k)}{k^2/2m}, \quad \text{where } \beta = \frac{1}{kT},$$

With the above $S(k\omega)$ this sum rule becomes:

$$\omega_0(k) = \left(\frac{k^2}{2m} / S(k)\right) \coth \left(\frac{1}{2}\, \beta\ \omega_0(k)\right) .$$

If $\frac{1}{2}\, \beta\omega_0(k) >> 1$, which is certainly true for the temperature and energy ranges we are working with, this sum rule becomes

$$\omega_0(k) = \frac{k^2}{2m\ S(k)} .$$

Thus the structure factor is determined by the dispersion relation which we do not know. Actually, we could calculate S(k). In his paper, Puff derives a sum rule which provides an integral equation for S(k). However, as will be shown in the next section, S(k) is not needed for comparison with experiment as S(kω) suffices. Therefore, we will not try to calculate S(k).

4. Relation to Cross Sections.

If particles are scattered from the many body system then the scattering cross section is given by

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \frac{M^2}{8\pi^3}\,\frac{P_F}{P_I}\,V_k^2\, S(k\omega) \qquad \text{(Van Hove)}\ ,$$

where it is assumed that the Born approximation applies. M is the mass of the particle being scattered, P_I is the initial momentum, P_F the final momentum, with energy transfer between ω and ω + dω and scattering angle dΩ. $V_k = \int e^{ik\cdot r}\, V(r)\, d^3r$ and ħ = 1.

If we integrate over all energy transfers

$$\frac{d\sigma}{d\Omega} = \int_0^\infty d\omega\, \frac{d^2\sigma}{d\omega\, d\Omega} = \frac{M^2}{8\pi^3}\,\frac{P_F}{P_I}\,V_k^2\, S(k)N\ .$$

Thus we see that if the scattering cross section is measured as a function of the energy transfer ω for a fixed scattering angle, the cross section should have a peak at those ω corresponding to the collective mode. If the angular distribution of the scattered particles is measured without specifying energy transfer, then $S(k)$ is determined.

We should mention that since in this work we required zero damping the peak in $S(k\omega)$ is infinitely high. If the problem were done more carefully, for example, if more diagrams were included in the evaluation of $\overline{V}$, the damping would not be zero and the peak would have finite height.

Normally if X-rays are scattered from the system, then the observed cross section is

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma_F}{d\Omega} S(\vec{k}) , \tag{3.3}$$

where $d\sigma_F/d\Omega$ is the differential scattering cross section for X-rays and a single electron. At energies $<< mc^2$, where m is the mass of an electron, $d\sigma_F/d\Omega$ reduces to the Thomson cross section $d\sigma_T/d\Omega$.

In usual X-ray scattering experiments, the energy transfer is small compared with the experimental resolution, and the observed cross section does not depend on the energy transfer. However, since we know more about $S(k\omega)$ than about $S(k)$, it is more convenient to look at the differential cross section with respect to the energy. Since the derivation of the Thomson scattering cross section is independent of the frequency we have

$$\frac{d\sigma}{d\Omega\, d\omega} = \frac{d\sigma_T}{d\Omega} S(\vec{k}\omega) \qquad ;$$

$$\frac{d\sigma_T}{d\Omega} = \frac{1}{2} \left(\frac{e^2}{mc^2}\right)^2 (2 - \sin^2 \theta) \; .$$

The cross section should show a peak at the frequency of the scattering X-ray which corresponds to ω_0, the predicted collective frequency. Experimentally, this might be determined from the Mossbauer effect.

CHAPTER IV

Hubbard's Solution for a Uniform Gas[11]

There are some important reasons for including the solution for a uniform gas in our discussion. The solution for the uniform gas guided the approximations used in the solution of the more general case. Furthermore, the general solution must reduce to the free gas solution when the external field goes to zero. Also, it is interesting to see how much simpler the problem is when there is no external field.

Consider now a many body system of electrons with no external forces present. The interaction $v(\vec{x}-\vec{x}')$ is the Coulomb interaction. In Chapter II it was found that

$$(2.25)\quad \Delta E = \frac{i\hbar}{2}\int_0^\lambda \frac{d\lambda}{\lambda}\int dx_1 \int dx_1'\ \delta(t_1)\ \overline{V}(x_1,x_1')\ V(x_1',x_1)$$

where

$$(2.20)\quad V(x_1',x_1) = v(x_1'-x_1) + \int V^*(x_1',x'')\ V(x'',x_1)\ dx''$$

$$v(x_1'-x_1) = v(\vec{x}_1'-\vec{x}_1)\ \delta(t_1'-t_1)$$

and

$$(2.27)\quad V^*(x',x) = \int \overline{V}(x',x'')\ v(x''-x)\ dx'' ,$$

and

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[11] J. Hubbard, Proc. of the Royal Soc. (London) A243 (1958) 336-351.

$$(2.26) \qquad \overline{V}(x',x) = \sum_{\Gamma \neq \Gamma_0}^{\text{proper}} \overline{W}(x',x\Gamma) \; .$$

In the absence of any external field, V, V^* and $\overline{V}$ are functions of only the differences in their arguments. Therefore equation (2.20) can be solved immediately by introducing the Fourier transforms of V, V^* and $\overline{V}$:

$$(4.1) \quad V(x',x) = \frac{1}{2\pi} \int d\vec{k} \int d\omega \, V(\vec{k},\omega) \, e^{i\vec{k}\cdot\overrightarrow{(x'-x)}+i\omega(t'-t)} .$$

The definitions for $V^*(\vec{k},\omega)$ and $\overline{V}(\vec{k},\omega)$ are similar. Equations (2.20) and (2.27) become

$$(4.2) \qquad V(\vec{k},\omega) = v(\vec{k}) + V^*(\vec{k},\omega) \, V(\vec{k},\omega)$$

$$(4.3) \qquad V^*(\vec{k},\omega) = v(\vec{k}) \, \overline{V}(\vec{k},\omega)$$

$$(4.4) \qquad v(k) = \frac{4\pi \, e^2}{k^2} \; ,$$

which is the Fourier transform of the Coulomb potential.

Equation (4.2) can be solved immediately.

$$(4.5) \qquad v(\vec{k},\omega) = \frac{v(\vec{k})}{1 - V^*(\vec{k},\omega)} \; .$$

The expression for ΔE becomes

$$(4.6) \qquad \Delta E = \frac{i\hbar}{4\pi n} \int_0^{\lambda} \frac{d\lambda}{\lambda} \int \frac{d\vec{k}}{(2\pi)^3} \int d\omega \, \frac{V^*(k,\omega)}{1 - V^*(k,\omega)}$$

where we have divided by the number of particles in the system and n is the particle density.

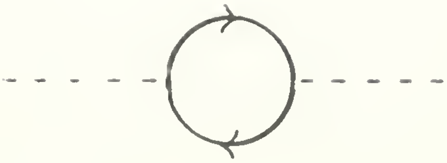
Writing $V'(\vec{k},\omega) = A(\vec{k},\omega) + i\sum(\vec{k},\omega)$,

$$(4.7) \quad \Delta E = \frac{\hbar}{4\pi n}\int_0^\lambda \frac{d\lambda}{\lambda}\int\frac{d\vec{k}}{(2\pi)^3}\int d\omega\,\frac{-\sum(\vec{k},\omega)}{[1-A(\vec{k},\omega)]^2+\sum^2(\vec{k},\omega)}$$

From (2.26) we have

$$(4.8) \qquad \overline{V}(\vec{k},\omega) = \sum_{\Gamma\neq\Gamma_0}^{\text{proper}} \overline{W}(\vec{k},\omega)$$

where the sum is over all proper polarization parts. This sum is approximated by its leading term, that corresponding to the simplest of all polarization parts shown in the following diagram.



The expression for $\overline{W}$ corresponding to this diagram is

$$(4.9) \qquad \overline{W}(x',x) = -\frac{1}{i\hbar}\,S(x',x)\,S(x,x') .$$

For a free gas

$$(4.10) \quad S(x',x) = \theta(t'-t)\sum_k^{\text{unocc}} e^{(i\vec{k}\cdot(\overrightarrow{x'-x})-\frac{i}{\hbar}E_k(t'-t))} - \theta(t-t')\sum_k^{\text{occ}} e^{(i\vec{k}\cdot(\overrightarrow{x'-x})-\frac{i}{\hbar}E_k(t'-t))},$$

where $E_k = \hbar^2k^2/2m$.

Substituting (4.10) into (4.9) we get

$$(4.11)\quad \overline{W}(x'-x) = \frac{1}{i\hbar}\Big[\theta(t'-t)\sum_{k'}^{\text{unocc}}\sum_{k''}^{\text{occ}} \cdot e^{i(\overrightarrow{k'-k''})\cdot(x'-x)-\frac{i}{\hbar}(E_{k'}-E_{k''})(t'-t)}$$

$$+\ \theta(t-t')\sum_{k'}^{\text{occ}}\sum_{k''}^{\text{unocc}} e^{[i(\overrightarrow{k'-k''})\cdot(\overrightarrow{x'-x})-\frac{i}{\hbar}(E_{k'}-E_{k''})(t'-t)]}\Big]$$

$\overline{W}(x'-x)$ is Fourier transformed to give $\overline{W}(\vec{k},\omega)$. Then $V^*(k,\omega)$ is derived by multiplying $\overline{W}(\vec{k},\omega)$ by $v(\vec{k}) = \frac{4\pi e^2}{k^2}$. The result is

$$(4.12)\quad V^*(\vec{k},\omega) = \frac{4\pi e^2}{m}\sum_{k'} N_{k'}\frac{P}{(\omega-\frac{\hbar}{m}k\cdot k')^2-\frac{\hbar^2k^4}{4m^2}}$$

$$-\ \frac{i}{\hbar}\frac{4\pi^2e^2}{k^2}\sum_{k'} N_{k'}(1-N_{k'+k})\Big[\delta\Big\{\frac{E_{k'+k}-E_{k'}}{\hbar}-\omega\Big\}$$

$$+\ \delta\Big(\frac{E_{k'+k}-E_{k'}}{\hbar}+\omega\Big)\Big]$$

where P means principal part and $N_k = \begin{cases} 1 \text{ if state } k \text{ is occupied} \\ 0 \text{ " " " not "} \end{cases}$.

The real part of this expression is A and the imaginary part is Σ.

Letting $x = k/k_F$ and $y = \hbar\omega/E_F$, it is found that for small x and for $y >> x(x+2)$

$$\Sigma(x,y) = 0$$

$$A(x,y) = \frac{y_p^2}{y^2}$$

$$y_p = \frac{\hbar\omega_p}{E_F}, \qquad \omega_p = \sqrt{\frac{4\pi n e^2}{m}}$$

Thus $A(x,y) = 1$ implies $y = y_p$ and the frequency equals the plasma frequency.

Before leaving this section, it is interesting to compare equation (4.6) for the energy shift for a uniform gas with equation (2.34) which is the energy shift for a general system.

$$(2.34) \quad \Delta E = \frac{i\hbar}{4\pi} \int_0^{\lambda} \frac{d\lambda}{\lambda} \int d\omega' \frac{\sum_i h_i(\omega')\, \mu_i(\omega')}{1 - \mu_i(\omega')}$$

where the μ_i are the eigenvalues of the homogeneous integral equation

$$(2.33) \quad \mu_i(\omega')\, \phi_i(\vec{x},\omega') = \int V^*(\vec{x},x',\omega')\, \phi_i(\vec{x}',\omega')\, dx' .$$

We see that for a uniform gas, the eigenvalue $\mu_i = \mu(\vec{k})$ is just the Fourier transform of $V^*(\vec{x},x',\omega')$, and the eigenfunctions $\phi_i(\vec{x},\omega') = \phi(\vec{k},\vec{x},\omega')$ are just plane waves or weighted spherical averages, i.e. free spherical waves.

CHAPTER V

The Solution for a Dense Electron Gas in an External Potential - General Remarks

It was shown in Chapter II that the information about collective modes is contained in the eigenvalues $\mu_i(\omega)$ of the integral equations

$$(2.33)\quad \mu_i(\omega)\phi_i(\vec{x},\omega) = \int V^*(\vec{x},\vec{x}',\omega)\phi_i(\vec{x}',\omega)\, dx'$$

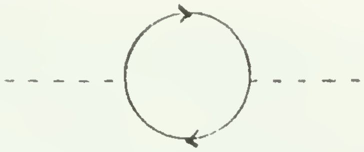
$$\mu_i(\omega)\chi_i(\vec{x},\omega) = \int V^*(\vec{x}',\vec{x},\omega)\chi_i(\vec{x}',\omega)\, dx'$$

where

$$(2.27)\quad V^*(x',x) = \int \overline{V}(x',x'')\, v(x''-x)\, dx''$$

$$(5.1)\qquad v(x''-x) = \frac{\delta(t''-t)e^2}{|\vec{x''-x}|}$$

and $\overline{V}$ was defined as the sum of proper polarization parts. (See Chapter II, Sections 5 and 6). For the calculation of $\overline{V}$, we shall keep only the leading term - the term that corresponds to the simplest of polarization parts:



It can be shown that $\overline{V}$ is a rapidly converging series for a weak interaction v or a very dense gas. Therefore, the keeping of only the leading term should be a good approximation for a high density electron gas. This approximation is often referred to in the literature as the random phase approximation; sometimes it is called the pair approximation. We saw that it was quite successful in predicting the collective motion for a free gas.

Therefore

$$(5.2) \qquad \bar{V}(x',x) = -\frac{1}{i\hbar} S(x',x)\, S(x,x')$$

where

$$(5.3) \quad S(x',x) = \theta(t'-t) \sum_{k}^{\text{unocc}} u_k(x')\, \bar{u}_k(x) - \theta(t-t') \sum_{k}^{\text{occ}} u_k(x')\, \bar{u}_k(x)$$

where θ is the step function and the $u_k(x)$ were defined in equation (2.6).

$$(2.6) \quad \left[\frac{p^2}{2m} + U(\vec{x}) + V(\vec{x})\right] u_k(\vec{x}) = E_i u_k(\vec{x}) \ .$$

$U(\vec{x})$ is the external potential and $V(\vec{x})$ is the self-consistent field. In the random phase approximation $V(\vec{x})$ is the Hartree field. Henceforth, we will assume $V(\vec{x})$ known and refer to the sum of $U(\vec{x})$ and $V(\vec{x})$ as $U(\vec{x})$.

From (5.2) and (5.3) we have

$$(5.4) \quad \bar{V}(x',x) = \frac{1}{i\hbar} \Big[\Big(\sum_{k}^{\text{unocc}} u_k(x')\, \bar{u}_k(x) \sum_{i}^{\text{occ}} u_i(x)\, \bar{u}_i(x')\Big) \cdot \theta(t'-t) + \theta(t-t') \sum_{i}^{\text{unocc}} u_i(x) \bar{u}_i(x') \sum_{k}^{\text{occ}} u_k(x')\, \bar{u}_k(x)\Big)\Big]$$

Now,

$$(5.5)\quad \sum_{i}^{occ} u_i(x)\,\bar{u}_i(x') = e^{-i\frac{H(t-t')}{\hbar}}\,\rho(\vec{x},\vec{x}\,')$$

where $H = p^2/2m + U$ and $\rho(\vec{x},\vec{x}\,')$ is the Dirac density matrix.

We will discuss two ways for evaluating $\bar{V}(x',x)$ and hence $\mu(\omega')$. Method II is an approximation for the density operator which is valid when the potential $U(x)$ is slowly varying. Method I couples a canonical transformation with a variational principle for a Green's function. These two methods are discussed in detail in the next two chapters.

In order to solve the integral equations (2.33) for the eigenvalues we can make use of a variational principle[12]

$$(5.6)\quad \mu_i(\omega') = \frac{\int \chi_i(\vec{x})\, V^*(\vec{x},\vec{x}\,',\omega')\, \phi_i(\vec{x}\,')\, d\vec{x}\, d\vec{x}\,'}{\int \phi_i(\vec{x})\, \chi_i(\vec{x})\, d\vec{x}}$$

in which $\mu_i(\omega')$ is stationary with respect to small variations in $\chi(x)$ and $\phi(x)$.

We will restrict our attention to the lowest eigenvalue which we will denote by μ_1.

In order to choose the trial functions $\phi(x)$ and $\chi(x)$ we can be guided by the following considerations:

(1) In the free electron gas the eigenfunctions were plane waves.

(2) The lowest eigenfunctions should be spherically symmetric.

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[12] Lovitt, W. V., Linear Integral Equations, New York, McGraw-Hill (1924).

(3) Our problem involves a slowly varying external potential.

(4) We will assume the external potential to be spherically symmetric.

Therefore, the following trial functions were used:

$$\chi(\vec{x}) = e^{-\alpha|\vec{x}|}$$

$$\phi(x') = e^{-\beta|\vec{x}'|}$$

where α and β are complex and their real parts are non-negative.

Using these functions, $\mu_1(\omega')$ will be calculated explicitly by the two different methods referred to above. Then from $\mu_1(\omega')$ we will determine whether any undamped collective modes exist, and if so, at what frequency.

CHAPTER VI

The Solution for a Dense Electron Gas in an External Potential - Method I

1. The Solution Expressed in Terms of a Green's Function.

Referring back to Chapter V, we see that to evaluate $\mu(\omega')$ we must know $\bar{V}(x',x)$. To do this we must evaluate $\sum_{i}^{occ} u_i(x)\bar{u}_i(x')$.

We can rewrite $\sum_{i}^{occ} u_i(x)\bar{u}_i(x')$ in the following form:

$$\sum_{i}^{occ} u_i(x)\bar{u}_i(x') = 2\langle x \mid e^{-itH}\, \theta(E_F-H) \mid x'\rangle$$

where $t = t-t'$, and H is the hamiltonian operator.

The factor of 2 is added to account for spin.

Also,

$$\sum_{k}^{unocc} u_k(x')\bar{u}_k(x) = 2\langle x' \mid e^{itH}\, \theta(H-E_F) \mid x\rangle$$

As stated in Chapter V, we will use the trial functions

$$\chi(x_1) = e^{-\alpha|r_1|}$$

$$\phi(x) = e^{-\beta|r|}$$

Define $\psi(r_2)$ to be $v \cdot \phi$

$$v(r_2,r) = \frac{q^2}{|r-r_2|}$$

$$\psi(r_2) = q^2 \int \frac{e^{-\beta|r|}}{|r-r_2|}\, d^3r\ .$$

After substituting into equation (5.6) and taking the Fourier transform with respect to t we have

$$(6.1)\quad \mu(\omega') = \frac{(\alpha+\beta)^3}{i\hbar 8\pi} \int dt\ \theta(-t) e^{-i\omega' t} \int d^3x_1\ d^3x_2$$

$$\cdot \{\chi(x_1)\psi(x_2)\langle x_1 |\ e^{\frac{it}{\hbar}(E_F-H)}\ 2\theta(E_F-H) |\ x_2\rangle$$

$$\cdot\ \langle x_2 |\ e^{-\frac{it}{\hbar}(E_F-H)} 2\theta(H-E_F) |\ x_1\rangle \}$$

$$+ \frac{(\alpha+\beta)^3}{i\hbar\ 8\pi} \int dt\ \theta(t)\ e^{-i\omega' t} \int d^3x_1\ d^3x_2$$

$$\cdot \{\chi(x_1)\psi(x_2)\ \langle x_2 |\ e^{-\frac{it}{\hbar}(E_F-H)} 2\theta(E_F-H) |\ x_1\rangle$$

$$\cdot\ \langle x_1 |\ e^{\frac{it}{\hbar}(E_F-H)} 2\theta(H-E_F) |\ x_2\rangle \}$$

where we have multiplied and divided by $e^{itE_F/\hbar}$.
The first term is the direct one; the second is the exchange term.

The expression $\mu(\omega')$ must be stationary with respect to α and β.

For ease in calculation we can rewrite equation (6.1) as

$$(6.2)\quad \mu(\omega') = \operatorname*{stat}_{\alpha,\beta} \frac{(\alpha+\beta)^3}{i\hbar 8\pi} \int dt\, e^{-i\omega' t}$$

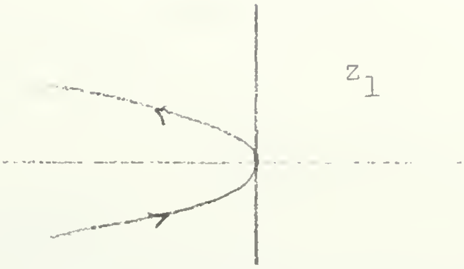
$$\cdot\{\theta(t)\,\mathrm{Tr}\,[\chi,\, e^{-i(E_F-H)\frac{t}{\hbar}}\, 2\theta(E_F-H)\psi\, e^{-i(H-E_F)\frac{t}{\hbar}}\, 2\theta(H-E_F)]$$

$$+\,\theta(-t)\,\mathrm{Tr}\,[\chi\, e^{-\frac{it}{\hbar}(H-E_F)}\, 2\theta(E_F-H)\psi\, e^{\frac{it}{\hbar}(H-E_F)}\, 2\theta(H-E_F)]\}$$

Now,

$$2\langle x_1|\, e^{\frac{it}{\hbar}(E_F-H)}\, \theta(E_F-H)\,|x_2\rangle = 2\,\frac{1}{2\pi i} \int \langle x_1|\frac{1}{z_1+E_F-H}|x_2\rangle e^{-\frac{it}{\hbar}z_1}\, dz_1$$

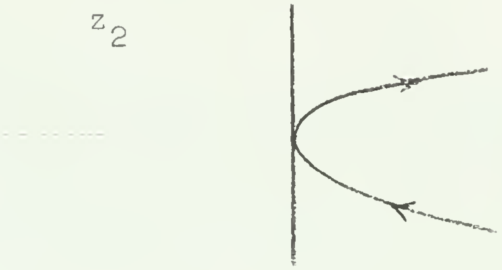
with the z_1 integration in the complex z_1 plane along the following path:



$\frac{1}{z_1+E_F-H}$ is the Green's function operator for a system whose Hamiltonian is H.

$$2\langle x_2|e^{it(H-E_F)}\theta(H-E_F)|x_1\rangle = -\,\frac{2}{2\pi i}\int\langle x_2|\frac{1}{z_2+E_F-H}|x_1\rangle e^{\frac{it}{\hbar}z_2}\, dz_2$$

The path of integration in the complex z_2 plane is:



Substituting into equation (6.2),

$$(6.3)\quad \mu(\omega') = \underset{\alpha\ \beta}{\text{stat}} \frac{(\alpha+\beta)^3}{-i\hbar 8\pi^3} \int dt\, e^{-i\omega' t} \int dz_1\, dz_2$$

$$\cdot\{\theta(t)\ \mathrm{Tr}\ [\chi,\ e^{+\frac{it}{h}z_1} \frac{1}{z_1+E_F-H}\ \psi\ e^{-\frac{it}{h}z_2} \frac{1}{z_2+E_F-H}]$$

$$+\ \theta(-t)\ \mathrm{Tr}\ [\chi\ e^{-\frac{it}{h}z_1} \frac{1}{z_1+E_F-H}\ \psi\ e^{\frac{it}{h}z_2} \frac{1}{z_2+E_F-H}]\}$$

which is the same as

$$(6.4)\ \mu(\omega') = \underset{\alpha\ \beta}{\text{stat}} \frac{(\alpha+\beta)^3}{-i\hbar 8\pi^3} \int dz_1\, dz_2\ \mathrm{Tr}\ [\chi \frac{1}{z_1+E_F-H}\ \psi\ \frac{1}{z_2+E_F-H}]$$

$$\cdot[\int_0^\infty e^{-i\omega' t}\, e^{itz_1/\hbar\ -itz_2/\hbar}\, dt$$

$$+\int_{-\infty}^0 e^{i\omega' t}\, e^{-itz_1/\hbar}\, e^{itz_2/\hbar}\, dt]\ .$$

Combining terms and integrating with respect to z gives:

$$(6.5)\quad \mu(\omega') = \underset{\alpha\ \beta}{\text{stat}} \frac{(\alpha+\beta)^3}{8\ \pi^3\ \hbar} \int dz_1\, dz_2\ \{\mathrm{Tr}\ [\chi \frac{1}{z_1+E_F-H}\ \psi\ \frac{1}{z_2+E_F-H}]$$

$$\cdot\ [\frac{1}{z_1-z_2+\omega'} + \frac{1}{z_1-z_2-\omega'}\ ]\}$$

where

$$(6.6)\quad \mathrm{Tr}\ [\chi \frac{1}{z_1+E_F-H}\ \psi\ \frac{1}{z_2+E_F-H}\ ]$$

$$= \int d^3x_1\, d^3x_2\ \chi(x_1)\psi(x_2)\ \langle x_1|\frac{1}{z_1+E_F-H}|x_2\rangle\ \langle x_2|\frac{1}{z_2+E_F-H}|x_1\rangle$$

2. Evaluation of the Green's Function.

For an arbitrary potential, we do not know the explicit closed form for

$$\langle x_1 \mid \frac{1}{z_1+E_F-H} \mid x_2 \rangle ,$$

$$H = \frac{p^2}{2m} + V$$

However, we can make use of a variational principle.

$$\frac{1}{z+W} = \underset{G}{\text{stat}}\ 2G - G(z+W)G$$

so

$$\langle x_1 | \frac{1}{z_1+E_F-H} | x_2 \rangle = \underset{G_1}{\text{stat}} \langle x_1 | (2G_1 - G_1(z_1+E_F-H)G_1) | x_2 \rangle$$

The problem now is to find a trial G_1.

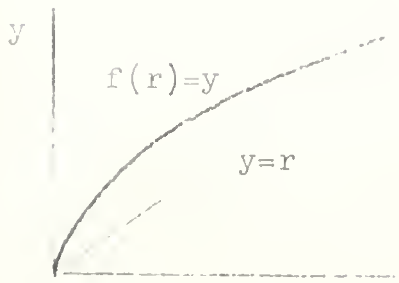
We know that if V = 0, then

$$\langle x_1 | G_1 | x_2 \rangle = -\frac{m}{2\pi\hbar^2} \frac{e^{\pm ik_1 |r_1-r_2|}}{|r_1 - r_2|}$$

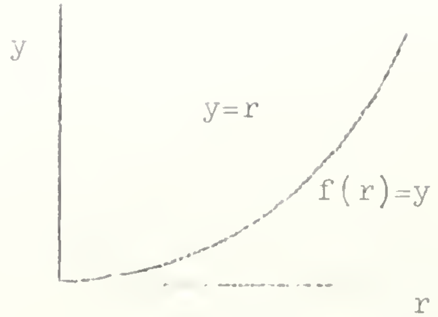
$$k_1 = \sqrt{\frac{(z_1+E_F)2m}{\hbar^2}}$$

To find $\langle x_1 | G_1 | x_2 \rangle$ when $V \neq r$ we try to find a canonical transformation from the system where $V \neq 0$ to a system where $V = 0$. The simplest canonical transformation to try is one which transforms only the spatial part and leaves the momentum alone. If we assume V to be spherically symmetric we can restrict the transformation to $f(|r|)$.

To visualize a transformation from a space with V(r) to one where V(r) equals zero, we can imagine a new space where |r| is stretched or compressed according to whether V is repulsive or attractive but with V(r) equal to zero. Also the origin and the point at infinity must be unchanged under f. The graphs below illustrate these general features that f(|r|) must possess.



V repulsive



V attractive

Since, in this new space V = 0, the Green's function is given by

$$\langle x_1|G_1|x_2\rangle = - \frac{m}{2\pi h^2} \frac{e^{\pm ik_1|f(r_1)-f(r_2)|}}{|f(r_1)-f(r_2)|} \frac{df}{dr_1} \frac{df}{dr_2}$$

where we have replaced r by f(r) in the G for V = 0 and multiplied by the Jacobian of the transformation.

Obviously, there are many functions f(r) with these general properties. The precise f(r) (which may still not be unique) would be determined from the specific V in question. If we could calculate f(r) directly from a knowledge of the potential $V(r)$ the Green's function would be determined.

However, for any general V we cannot calculate $f(r)$ exactly. It is not necessary to do this however. We can choose any $f(r)$ with the general properties described above and insert into this $f(r)$ parameters to be determined from the variational principle for G_1. From now on, we will understand f to be a function of r and these unknown parameters.

For example, suppose $V = b\, e^{-a|r|}$.

We can use $f(r) = \frac{|r| e^{a|r|} + \varepsilon |r|}{e^{a|r|}}$, where the unknown parameter ε is complex to allow for a phase shift. We note that: $f(r) \rightarrow 0$ as $r \rightarrow 0$

and $r(r) \rightarrow \infty$ as $r \rightarrow \infty$.

This particular form for $f(r)$ was chosen because it satisfies the required general properties and somewhat resembles the form of $V(r)$.

Returning to the variational principle for G_1 we shall use as a trial G_1:

$$(6.7) \quad \langle x_1 | G_1 | x_2 \rangle = - \frac{m}{2\pi\hbar^2} \frac{\sin (k_1 |f_1(r_1) - f_1(r_2)|}{|f_1(r_1) - f_1(r_2)|} = G_1(x_1, x_2)$$

$$k_1 = \sqrt{\frac{(z_1 + E_F) 2m}{\hbar^2}}$$

We have omitted the Jacobian because we needed not the exact transformation but only a form to use as a trial function. The sine function is used because it is that linear combination of e^{ikr}/r and e^{-ikr}/r which is finite at the origin.

$$\langle x_1 | G_1 (z_1+E_F-H) G_1 | x_2 \rangle$$

$$= \int d^3x_3 \; G_1(x_1,x_3)(z_1+E_F+ \frac{\hbar^2}{2m} \nabla_3^2 - V(r_3) \; G_1(x_3,x_2)$$

We want to evaluate

$$\langle x_1 | G_1 (z_1+E_F-H) G_1 | x_2 \rangle$$

$$= \int G_1(x_1,x_3)(z+E_F+ \frac{\hbar^2}{2m} \nabla_3^2 - V(r_3)) \; G_1(x_3,x_2) \; d^3x_3 \; .$$

$\frac{\hbar^2}{2m} \int G(x_1,x_3)\nabla_3^2 G(x_3,x_2) d^3x_3$ can be simplified by using Green's Theorem.

$$\int \mathrm{div}_3 \; G_{(1,3)} \; \mathrm{grad}_3 \; G_{(3,2)} \; d^3x_3 = \int G_{(1,3)} \mathrm{grad}_3 G_{(3,2)} dS_3$$

$$= \int \mathrm{grad}_3 \; G_{(1,3)} \cdot \mathrm{grad}_3 \; G_{(3,2)} \; d^3x_3 + \int G_{(1,3)} \nabla_3^2 \; G_{(3,2)} d^3x_3$$

Because of the form of G, the surface integral (the surface is at infinity) goes to zero and we are left with

$$(6.8) \qquad - \frac{\hbar^2}{2m} \int \nabla_3 \; G_1(x_1,x_3) \cdot \nabla_3 G_1(x_3,x_2) \; d^3x_2$$

It is straightforward to evaluate the gradients and to take the dot product. We leave the evaluation of the integral to numerical methods.

Let us denote by $K_1(x_1,x_2)$ the following sum:

$$(6.9)\quad K_1(x_1,x_2) = \int G_1(x_1,x_3)\ (z_1 + E_F)G_1(x_3,x_1)r_3^2\ dr_3 d\cos\theta_3$$

$$- \int G_1(x_1,x_3)\ V(r_3)G_1(x_3,x_2)\ d^3x_3$$

$$- \frac{\hbar^2}{2m}\int \nabla_3 G_1(x_1,x_3)\cdot\nabla_3 G_1(x_3,x_2)\ d^3x_3\ .$$

Letting $R = f^2(r_1) + f^2(r_2) - 2f(r_1)f(r_2)\cos(\theta_1-\theta_2)$,

$$(6.10)\ \langle x_1|\frac{1}{z_1+E_F-H}|x_2\rangle = \text{stat}_f(2G_1(x_1,x_2)-K_1(x_1,x_2))$$

$$= \text{stat}_f\left(-\frac{m}{\pi\hbar^2}\ \frac{\sin(k_1R^{1/2})}{R^{1/2}} - K_1(x_1,x_2)\right)$$

Also,

$$\langle x_2|\frac{1}{z_2+E_F-H}|x_1\rangle = \text{stat}_{f_2}\langle x_2|2G_2-G_2(z_2+E_F-H)G_2)|x_1\rangle$$

Try

$$\langle x_2|G_2|x_1\rangle = G_2(x_2,x_1) = -\frac{m}{2\pi\hbar^2}\ \frac{\sin(k_2|f(r_2)-f(r_1)|}{|f(r_1) - f(r_2)|}$$

with

$$k_2 = \sqrt{\frac{(z_2+E_F)2m}{\hbar^2}}$$

As before,

$$(6.11)\quad \langle x_2|G_2(z_2+E_F-H)G_2|x_1\rangle$$

$$= \int d^3x_3\ G_2(x_2,x_3)\ (z_2+E_F + \frac{\hbar^2}{2m}\nabla_3^2 - V(r_3))G_2(x_3,x_1)$$

Define $K_2(x_2,x_1)$ as

$$(6.12)\quad K_2(x_2,x_1) = -\frac{\hbar^2}{2m}\int \nabla_3 G_2(x_2,x_3)\cdot\nabla_3 G_2(x_3,x_1)\,2\pi r_3^2\,dr_3\,d\cos\theta$$

$$+\int G_2(x_2,x_3)(z_1+E_F)G_2(x_3,x_1)\,2\pi r_3^2\,dr_3\,d\cos\theta$$

$$-\int G_2(x_2,x_3)V(r_3)G_2(x_3,x_1)\,d^3x_3$$

so that

$$(6.13)\quad \langle x_2|\frac{1}{z_2+E_F-H}|x_1\rangle = \mathrm{stat}_f(2G_2(x_2,x_1)-K_2(x_2,x_1))$$

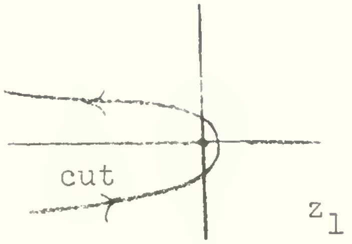
$$= \mathrm{stat}_f\left[\frac{-m}{\pi\hbar^2}\;\frac{\sin(k_2R^{1/2})}{R^{1/2}} - K_2(x_2,x_1)\right]$$

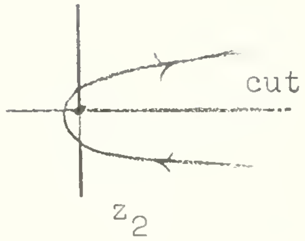
where $R = f^2(r_1) + f^2(r_2) - 2f(r_1)f(r_2)\cos(\theta_1-\theta_2)$.

Expressions (6.10) and (6.13) are substituted into equation (6.5).

Because of the way in which k_1 and k_2 are defined, the factors $z_1^{1/2}$ and $z_2^{1/2}$ occur. Therefore we must define branch cuts in the z_1 and z_2 planes before doing the integrations over z_1 and z_2. Mathematically, we are not restricted in making the branch cut. However physical arguments dictate that the cut correspond to the bound states. Actually, if we make the cuts in any other way, we find that $\mu(\omega')$ is identically zero which is not a physical solution.

Below are diagrams of the z_1 and z_2 planes which indicate the paths of integration and the branch cuts.





We now refer back to equation (6.5).

$$\chi(x_1) = e^{-\alpha|r_1|}$$

$$\psi(x_2) = \int \frac{e^{-\beta|r|}}{|r-r_2|} d^3r \ .$$

In equation (6.6) we have to integrate over $d^3r_1\ d^3r_2\ d^3r$. Let $d^3r_2\ d^3r \to 4\pi^2 r\ r_2\ dr_2\ dr\ |r-r_2|\ d|r-r_2|\ d\cos\theta_2$.

$$(6.14)\quad \mu(\omega') = \operatorname{stat}_{\alpha\beta f} \frac{(\alpha+\beta)^3}{2\pi} \int dz_1 dz_2 r_1^2 dr_1 d\cos\theta_1 g(r_1,r_2,\theta_1,\theta_2)$$

$$\cdot \frac{e^{-\beta\ r}}{|r-r_2|}\ r\ dr\ dr_2|r-r_2|d|r-r_2|d\cos\theta_2$$

where $g(r_1,r_2,\theta_1,\theta_2)$ encompasses all the terms in the integrand which are functions of only r_1 and r_2; i.e.

$$(6.15)\quad g(r_1,r_2,\theta_1,\theta_2) = e^{-\alpha r_1} \langle x_1|\frac{1}{z_1+E_F-H}|x_2\rangle\langle x_2|\frac{1}{z_2+E_F-H}|x_1\rangle$$

See equation (6.10) for $\langle x_1|\frac{1}{z_2+E_F-H}|x_2\rangle$ and see equation (6.13) for $\langle x_2|\frac{1}{z_2+E_F-H}|x_1\rangle$. The integration over $|r-r_2|$, r, and r_2 is:

$$\int_0^\infty dr_2 \int_{r_2}^\infty dr \int_{r-r_2}^{r+r_2} d|r-r_2| + \int_0^\infty dr_2 \int_0^{r_2} dr \int_{r_2-r}^{r_2+r} d|r-r_2|$$

The first term:

$$\int_0^\infty r_2\, dr_2 \int_{r_2}^\infty r\, dr \int_{r-r_2}^{r+r_2} d|r-r_2|\; |r-r_2|\; e^{-\beta\, r}\; g(r_1,r_2,\theta_1,\theta_2)$$

$$\cdot \frac{1}{|r-r_2|}\, d \cos\, \theta_2$$

The integration over $d|r-r_2|$ gives the factor $2r_2$. We now have

$$\int_0^\infty 2r_2^2\, dr_2\, d \cos\, \theta_2\; g(r_1,r_2,\theta_1,\theta_2) \int_{r_2}^\infty e^{-\beta r}\, r\, dr$$

$$\int_{r_2}^\infty e^{-\beta r}\, r\, dr = \frac{1}{\beta^2}\, e^{-\beta\, r_2} + \frac{r_2}{\beta}\, e^{-\beta\, r_2}$$

The second term:

$$\int_0^\infty r_2\, dr_2 \int_0^{r_2} r\, dr \int_{r_2-r}^{r_2+r} d|r-r_2|\; |r-r_2|\; e^{-\beta\, r}\; g(r_1,r_2,\theta_1,\theta_2)$$

$$\cdot \frac{1}{|r-r_2|}\, d \cos\, \theta_2 \,.$$

The integration over $d|r-r_2|$ equals $2r$.

$$\int_0^\infty r_2\, dr_2\, d \cos\, \theta_2\; g(r_1,r_2,\theta_1,\theta_2) \int_0^{r_2} 2r^2\, dr\, e^{-\beta\, r}$$

$$\int_0^{r_2} dr\, 2r^2\, e^{-\beta r} = -\frac{2e^{-\beta\, r_2}\, r_2^2}{\beta} - \frac{4r_2\, e^{-\beta\, r_2}}{\beta^2} - \frac{4e^{-\beta r_2}}{\beta^3} + \frac{4}{\beta^3}$$

Defining:

$$g_1(r_1,r_2,\theta_1,\theta_2) = g(r_1,r_2,\theta_1,\theta_2)\ \left(\frac{1}{\beta^2}\, e^{-\beta r_2} + \frac{r_2}{\beta}\, e^{-\beta r_2}\right)$$

$$g_2(r_1,r_2,\theta_1,\theta_3) = g(r_1,r_2,\theta_1,\theta_2)\ \left(- \frac{2e^{-\beta r_2}\, r_2^2}{\beta} - \frac{4r_2 e^{-\beta r_2}}{\beta^2} - \frac{4e^{-\beta r_2}}{\beta^3} + \frac{4}{\beta^3}\right) ,$$

$$(6.15)\quad \mu(\omega') = \operatorname{stat}_{\alpha\beta_f} \frac{(\alpha+\beta)^3}{2\pi} \int dz_1 \int dz_1 \int_0^\infty dr_1\ r_1^2 \cdot \int_{-\pi}^{\pi} \sin\theta_1 d\theta_1 \int_{-\pi}^{\pi} \sin\theta_2 d\theta_2$$
$$\cdot \left[\int_0^\infty 2r_2^2 g_1(r_1,r_2,\theta_1,\theta_2,z_1,z_2,f)\ dr_2 + \int_0^\infty r_2\ dr_2\ g_2(r_1,r_2,\theta_1,\theta_2,z_1,z_2,f)\right] .$$

We leave the remaining integrations to be done numerically. Then we must find the stationary value by varying α, β, and the parameters in the transformation f.

CHAPTER VII

The Solution for a Dense Electron Gas in an External Potential - Method II

1. An Approximation for the Modified Interaction for a Slowly Varying External Potential.

We saw in Chapter V that the solution of our problem depends upon calculating the eigenvalue $\mu_1(\omega')$ which was approximated by equation (5.6):

$$(5.6) \quad \mu_1(\omega') = \frac{\int \chi(\vec{x})\, V^*(\vec{x},\vec{x}',\omega')\, \phi(\vec{x}')\, d\vec{x}\, d\vec{x}'}{\int \phi(\vec{x})\, \chi(\vec{x})\, d\vec{x}}$$

where, for a spherically symmetric potential we decided to use

$$\chi(\vec{x}) = e^{-\alpha|\vec{x}|}$$

$$\phi(\vec{x}') = e^{-\beta|\vec{x}'|}$$

and V^* is the modified interaction. This expression for $\mu_1(\omega')$ must be stationary with respect to the complex parameters α and β. The modified interaction V^* is given by

$$(7.1) \quad V^*(x',x) = \int \overline{V}(x',x'')\, \frac{\delta(t''-t)q^2}{|\vec{x}''-\vec{x}|}\, dx''$$

It was shown in Chapter V that, in the random phase approximation, $\overline{V}$ is given by

$$(5.4)\quad \bar{V}(x',x) = \frac{1}{i\hbar}\Big[\Big(\sum_{k}^{\text{unocc}} u_k(x')\,\bar{u}_k(x) \sum_{i}^{\text{occ}} u_i(x)\,\bar{u}_i(x')\Big)\theta(t'-t)$$

$$+\,\theta(t-t')\sum_{i}^{\text{unocc}} u_i(x)\,\bar{u}_i(x') \sum_{k}^{\text{occ}} u_k(x')\,\bar{u}_k(x)\Big)\Big]$$

where $\theta(x) = 1\,,\quad x > 0$

$\qquad 0\,,\quad x < 0$

$\qquad \frac{1}{2}\,,\quad x = 0$

and $\sum_{i}^{\text{occ}} u_i(x)\,\bar{u}_i(x') = e^{-iH(t-t')/\hbar}\,\rho(\vec{x},\vec{x}')$

where $H = \frac{p^2}{2m} + U$

and $\rho(\vec{x},\vec{x}')$ is the Dirac density matrix.

If the potential $U(\vec{x})$ is slowly varying, we can approximate $\rho(\vec{x},\vec{x}')$ by:

$$(7.2)\quad \rho(\vec{x},\vec{x}') = -\frac{2}{h^3 2\pi i}\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} d\omega \int d^3p$$

$$\cdot\,\frac{e^{i\vec{p}\cdot(\vec{x}-\vec{x}')/\hbar}\;e^{-i\omega[E_F-\frac{p^2}{2m}+U(\underline{\vec{x}})]+\frac{i\omega^3\hbar^2}{24\,m}|\nabla U(\underline{x})|^2}}{\omega}$$

where $\underline{\vec{x}} = \frac{\overrightarrow{x+x'}}{2}$

This approximation is a corrected Thomas-Fermi model. If $\nabla u(x)$ is zero, then (7.2) is just the Thomas-Fermi result. A complete discussion of how this approximation is arrived at is to be found in Appendix A.

To find $e^{-iH(t-t')/\hbar}\rho(\vec{x},\vec{x}')$:

$$(7.3) \qquad \rho(\vec{x},\vec{x}') = \theta(E_F-H)\,\delta(x-x')$$

$$= -\frac{1}{2\pi i}\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \frac{e^{-i\omega(E_F-H)}}{\omega}\,d\omega\,\delta(\vec{x}-\vec{x}')$$

so that

$$(7.4) \quad e^{-iH(t-t')/\hbar}\rho(\vec{x},\vec{x}') = -e^{-iH(t-t')/\hbar}\frac{1}{2\pi i}$$

$$\cdot\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \frac{e^{-i\omega(E_F-H)}}{\omega}\,d\omega\,\delta(x-x').$$

Let $u = \omega - (t-t')/\hbar$ and $\omega = u + (t-t')/\hbar$. Then

$$(7.5) \quad e^{-iH(t-t')/\hbar}\rho(\vec{x},\vec{x}') = e^{-iE_F(t-t')/\hbar}$$

$$\cdot\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} \frac{e^{-iu(E_F-H)}}{u+(t-t')/\hbar}\,du\,\delta(x-x') \ .$$

For slowly varying $u(\vec{x})$ we can approximate (7.5) by

$$(7.6) \quad e^{-iH(t-t')/\hbar}\rho(\vec{x},\vec{x}') = \frac{-2}{h^3 2\pi i}\,e^{-iE_F(t-t')/\hbar}$$

$$\cdot\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon} d\omega \int d^3p\left[\frac{e^{i\frac{\vec{p}}{\hbar}\cdot(\vec{x}-\vec{x}')}\,e^{-i\omega(E_F-\frac{p^2}{2m}-U(\underline{x}))}}{\omega+(t-t')/\hbar}\right.$$

$$\left.\cdot\, e^{i\omega^3\hbar^2|\nabla U(\underline{x})|^2/24m}\right]$$

Also,

$$(7.7) \quad \sum_k^{\text{unocc}} u_k(x')\,\bar{u}_k(x) = e^{-iH(t'-t)/\hbar}[\delta(\vec{x}'-\vec{x}) - \rho(\vec{x}',\vec{x})]$$

and if $U(x)$ is slowly varying

$$(7.8)\quad e^{-iH(t'-t)/\hbar}\,\delta(\vec{x}'-\vec{x}) = e^{+iH(t-t')/\hbar}\,\delta(\vec{x}'-\vec{x})$$

$$= \frac{2}{h^3}\int e^{i\frac{t-t'}{\hbar}\left[\frac{p^2}{2m}+U(\underline{x})\right]+i\frac{(t-t')^3\hbar^2}{\hbar^3 24m}|\nabla U(\underline{x})|^2}\; e^{i\vec{p}\cdot(\vec{x}'-\vec{x})/\hbar}\, d^3p.$$

For the time being consider only the first term of $\overline{V}(x',x)$ since the second term differs only by an interchange of x and x'.

$$(7.9)\quad \overline{V}(x',x) = \frac{1}{i\hbar}\left[\theta(t'-t)\sum_{k}^{\text{unocc}} u_k(x')\,\bar{u}_k(x)\sum_{i}^{\text{occ}} u_i(x)\bar{u}_i(x')\right]$$

$$(7.10)\quad \overline{V}(x',x) = \frac{1}{i\hbar}\,\theta(t'-t)\, e^{-\frac{iH}{\hbar}(t-t')}\,\rho(\vec{x},\vec{x}')$$

$$\cdot\left[e^{+i\frac{H(t-t')}{\hbar}}\,\delta(\vec{x}'-\vec{x}) - e^{+i\frac{H(t-t')}{\hbar}}\,\rho(\vec{x}',\vec{x})\right].$$

Writing

$$\theta(t'-t) = \frac{-1}{2\pi i}\int_{-\infty+i\varepsilon}^{\infty+i\varepsilon}\frac{e^{-i\omega(t'-t)}}{\omega}\,d\omega\,,$$

using the aforementioned approximations (7.6) and (7.8), and taking the Fourier transform of $\overline{V}$ i.e.

$$\hbar\int e^{-i\omega'\left(\frac{t-t'}{\hbar}\right)}\,d\left(\frac{t-t'}{\hbar}\right)\,\overline{V}(x',x)\,,$$

and also letting $\vec{x} = \vec{r}_1$, $\vec{x}' = \vec{r}_2$ we get the following expression for $\overline{V}(\vec{r}_2,\vec{r}_1,\omega')$:

$$(7.11)\quad \overline{V}(\vec{r}_2,\vec{r}_1,\omega') = \frac{-1}{ih^6\pi^2}\int\Bigg\{\Bigg[e^{-iE_F\left(\frac{t-t'}{\hbar}\right)}$$

$$\cdot e^{-i\omega_1\left(E_F-\frac{p_1^2}{2m}-U\left(\frac{r_1+r_2}{2}\right)+\frac{i\omega_1^3\hbar^2}{24m}\left|\nabla U\left(\frac{r_1+r_2}{2}\right)\right|^2\right]}/[\omega_1+(\frac{t-t'}{\hbar})]\omega$$

$$\cdot e^{i(t-t')\left[\frac{p_2^2}{2m}+U\left(\frac{r_1+r_2}{2}\right)+\frac{i(t-t')^3\hbar^2}{\hbar^3\,24m}\left|\nabla U\left(\frac{r_1+r_2}{2}\right)\right|^2\right.}$$

$$\cdot e^{i\omega\hbar\left(\frac{t'-t}{\hbar}\right)}\;e^{-i\omega'\hbar\left(\frac{t-t'}{\hbar}\right)}\,d\omega_1\;d\omega\;d\left(\frac{t-t'}{\hbar}\right)\;d^3p_1\;d^3p_2$$

$$\cdot e^{\frac{ip_1\cdot(\vec{r}_1-\vec{r}_2)}{\hbar}+\frac{ip_2\cdot(\vec{r}_2-\vec{r}_1)}{\hbar}}\Bigg\}$$

$$+\frac{1}{ih^6\pi^2}\int_{-\infty+i\varepsilon}^{\omega'+i\varepsilon}d\omega\int_{-\infty}^{\infty}d^3p_1\;d^3p_2\;d\omega_1\;d\omega_2$$

$$\Bigg\{\cdot\Bigg[e^{\frac{ip_1\cdot(\vec{r}_1-\vec{r}_2)}{\hbar}+\frac{ip_2\cdot(\vec{r}_2-\vec{r}_1)}{\hbar}}\;e^{-i\omega_1\omega\hbar\;+i\omega'\hbar\omega_1}\Bigg]/\omega(\omega_1+\omega_2)]$$

$$\cdot\;e^{-i\omega_1\left[E_F-\frac{p_1^2}{2m}-U\left(\frac{r_1+r_2}{2}\right)\right]+\frac{i\omega_1^2\hbar^2}{24m}\left|\nabla U\left(\frac{r_1+r_2}{2}\right)\right|^2}$$

$$\cdot\;e^{-i\omega_2\left[E_F-\frac{p_2^2}{2m}-U\left(\frac{r_1+r_2}{2}\right)\right]+\frac{i\omega_2^3\hbar^2}{24m}\left|\nabla U(r_1+r_2)\right|^2]}\Bigg\}$$

$$-\frac{1}{ih^6\pi^2}\int_{\omega'}^{\infty}d\omega\int_{-\infty}^{\infty}d^3p_1\;d^3p_2\;d\omega_1\;d\omega_2$$

$$\Bigg\{\cdot\Bigg[e^{\frac{ip_1\cdot(\vec{r}_1-\vec{r}_2}{\hbar}+\frac{ip_2\cdot(\vec{r}_2-\vec{r}_1)}{\hbar}}\;e^{i\omega\omega_2\hbar\;-i\omega'\hbar\omega_2}\Bigg]/\omega(\omega_1+\omega_2)]$$

$$\cdot\;[e^{-i\omega_1\left[E_F-\frac{p_1^2}{2m}-U\left(\frac{r_1+r_2}{2}\right)\right]+\frac{i\omega_1^3\hbar^2}{24m}\left|\nabla U\left(\frac{r_1+r_2}{2}\right)\right|^2}$$

$$\cdot\;e^{-i\omega_2\left[E_F-\frac{p_2^2}{2m}-U\left(\frac{r_1+r_2}{2}\right)\right]+\frac{i\omega_2^3\hbar^2}{24m}\left|\nabla U\left(\frac{r_1+r_2}{2}\right)\right|^2]}\Bigg\}$$

We assume that $v(|\overrightarrow{r_1-r_2}|)$, the interaction between the particles, is the coulomb interaction, $v(|\overrightarrow{r_1-r_2}|) = \dfrac{q^2}{|r_1-r_2|}$

(7.12) $V^*(r_1,r,\omega') = \int \frac{q^2}{|r_2-r|} \overline{V}(r_2,r_1,\omega')\, dr_2$

and

(7.13) $\mu_1(\omega') = \frac{\int e^{-\alpha r_1} e^{-\beta r} V^*(r_1,r,\omega')\, d^3r_1\, d^3r}{\int e^{-\alpha r-\beta r}\, d^3r}$

2. A Sample Term of the Solution Expression as a Many Dimensional Integral.

Call $\mu_1(\omega') \int e^{-\alpha r} e^{-\beta r} d^3r = \bar{\mu}_1(\omega') = \frac{\mu_1(\omega')\, 8\pi}{(\alpha+\beta)^3}$

We now want to calculate $\overline{\mu}_1(\omega')$.

Since the different terms in $\overline{V}$ all involve the same integrations in r, r_1, r_2, p_1 and p_2 just look at the last term to do these integrals. Let

(7.14) $e^{-\alpha r_1} = \int d^3k_1 \frac{\phi(k_1)}{(2\pi)^3} e^{ik_1\cdot r_1}$

$$e^{-\beta r} = \int d^3k_2 \frac{\psi(k_2)}{(2\pi)^3} e^{ik_2\cdot r}$$

$$\phi(k_1) = \frac{8\pi\alpha}{(k_1^2+\alpha^2)^2}, \qquad \psi(k_2) = \frac{8\pi\beta}{(k_2^2+\beta^2)^2}.$$

Also, make the following substitutions:

(7.15)
$$\begin{aligned} \frac{\vec{r}_1+\vec{r}_2}{2} &= \vec{\rho}_1, & \vec{\rho}_1 + \vec{\rho}_3 &= \vec{r}_1 \\ \frac{\vec{r}_1-\vec{r}_2}{2} &= \vec{\rho}_3, & \vec{\rho}_1 - \vec{\rho}_3 &= \vec{r}_2 \\ \vec{r}_2 - \vec{r} &= \vec{\rho}_2, & \vec{\rho}_1 - \vec{\rho}_3 - \vec{\rho}_2 &= \vec{r} \end{aligned}$$

The Jacobian of this transformation is 2.

The last term of $\bar{\mu}_1(\omega')$ is

$$(7.16)\quad \bar{\mu}_1(\omega') = \int_{-\infty}^{\infty} d^3p_1\, d^3p_2\, d\omega_1\, d\omega_2\, d^3\rho_1\, d^3\rho_2\, d^3\rho_3\, d^3k_1\, d^3k_2$$

$$\cdot \int_{\omega'}^{\infty} d\omega \Bigg\{ -\frac{2q^2}{ih^6\pi^2} \left[\frac{e^{i\omega\omega_2\hbar - i\omega'\hbar\omega_2}}{\omega(\omega_1+\omega_2)} \quad \frac{1}{|\rho_2|} \quad \frac{\Phi(k_1)\ \psi(k_2)}{(2\pi)^3(2\pi)^3} \right.$$

$$\cdot\ e^{ik_1(\rho_1+\rho_3)}\ e^{ik_2(\rho_1-\rho_3-\rho_2)}\ e^{ip_1\cdot 2\rho_3/\hbar}\ e^{-ip_2\cdot 2\rho_3/\hbar}$$

$$\cdot\ e^{i\omega_1[E_F - \frac{p_1^2}{2m} - U(\rho_1)] + \frac{i\omega_1^3\hbar^2}{24m} |\nabla U(\rho_1)|^2}$$

$$\left. \cdot\ e^{-i\omega_2[E_F - \frac{p_2^2}{2m} - U(\rho_1)] + \frac{i\omega_2^3\hbar^2}{24m} |\nabla U(\rho_1)|^2} \right] \Bigg\}$$

The integral over ρ_2 is

$$(7.17)\qquad \int \frac{1}{|\rho_2|}\ e^{-i\vec{k}_2\cdot\vec{\rho}_2}\ d^3\rho_2 = \frac{4\pi}{k_2^2}$$

The integrals over p_1, p_2 and ρ_3 combine to the following

$$(7.18)\qquad \frac{-\pi^4\sqrt{\pi}(2m)^{3/2}\ \hbar^2}{(i)^{1/2}(\omega_1+\omega_2)^{3/2}}\quad e^{i\hbar^2|k_1-k_2|^2\omega_1\omega_2\ /8m(\omega_1+\omega_2)}$$

and the last term of $\bar{\mu}_1(\omega')$ becomes

$$(7.19)\qquad \int_{\omega'+i\varepsilon}^{\infty+i\varepsilon} d\omega \int_{-\infty}^{\infty} \frac{d\omega_1\ d\omega_2\ d^3\rho_1\ d^3k_1\ d^3k_2}{\omega(\omega_1+\omega_2)^{5/2}}$$

$$\cdot\ e^{i\omega_2\hbar - i\omega'\hbar\omega_2}\ \cdot\ \frac{q^2 8(2m)^{3/2}\hbar^3}{i^{3/2}h^6\ \sqrt{\pi}} \left[\frac{\alpha}{(k_1^2+\alpha^2)^2}\quad \frac{\beta}{(k_2^2+\beta^2)^2} \right. \cdot$$

$$\cdot \frac{e^{i\vec{K}_1\cdot\vec{\rho}_1}\, e^{i\vec{K}_2\cdot\vec{\rho}_1}}{k_2^2}\; e^{i|k_1-k_2|^2\hbar^2\omega_1\omega_2/8m(\omega_1+\omega_2)}$$

$$\cdot\; e^{-i\omega_1(E_F-U(\rho_1))+\frac{i\omega_1^3\hbar^2}{24m}|\nabla U(\rho_1)|^2}$$

$$\cdot\; e^{-i\omega_2(E_F-U(\rho_1))+\frac{i\omega_2^3\hbar^2}{24m}|\nabla U(\rho_1)|^2} \quad .$$

3. A Variational Principle is Introduced to Simplify the Integration.

We now consider the integration over ρ_1. If the form of the potential $U(\rho_1)$ is particularly simple (for example, linear in ρ_1) then the integration over ρ_1 is straightforward and not difficult. However, for many more complicated forms of $U(\rho_1)$ the integration can no longer be performed in closed form. Also, it is preferable to continue the problem without having to make a specific choice for $U(\rho_1)$ at this point in the calculation so that the final solution would be valid for any general $U(\rho_1)$ consistent with the initial assumptions of spherical symmetry and slow variation of U with ρ_1. To accomplish this, use was made of the following variational principle:

$$(7.20) \quad \int e^{-u(x)}\, W(x)\, dx = \int f(x)\omega(x)\, dx - \int u(x)\omega(x)f(x)\, dx$$
$$- \int f(x) \ln f(x)\, \omega(x)\, dx \; .$$

where the expression is stationary against variations in f.

To show the validity of this variational principle, take the variation of the right hand side and set it equal to zero, i.e.

$$0 = [\int f(x)\omega(x)\,dx - \int u(x)\omega(x)f(x)\,dx - \int f(x)\ln f(x)\omega(x)dx$$

$$0 = \int \delta f(x)\omega(x)\,dx - \int u(x)\omega(x)\,\delta f(x)\,dx -$$

$$- \int \delta f(x)\ln f(x)\,\omega(x)\,dx - \int \delta f(x)\omega(x)\,dx$$

$$0 = - \int u(x)\omega(x)\,\delta f(x)\,dx - \int \delta f(x)\ln f(x)\,\omega(x)\,dx$$

$$0 = - \int \omega(x)\,\delta f(x)[u(x) + \ln f(x)]\,dx$$

$\ln f(x) = -u(x)$,

$f(x) = e^{-u(x)}$ at the stationary point of the right hand side. With this value for $f(x)$ the right hand side is $\int e^{-u(x)}\omega(x)\,dx - \int u(x)\omega(x)e^{-u(x)}\,dx + \int e^{-u(x)}u(x)\omega(x)\,dx = \int e^{-u(x)}\,\omega(x)\,dx$ which is the same as the left hand side.

We want to calculate $\int e^{-u(\rho_1)}\omega(\rho_1)\,d^3\rho_1$ where $\omega(\rho_1) = e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{\rho}_1}$

$$u = - i(\omega_1+\omega_2)U(\rho_1) - \frac{i(\omega_1^3+\omega_2^3)\hbar^2|\nabla U(\rho_1)|^2}{24\,m}.$$

Assume $f = f(|\rho_1|, p_1 \ldots p_i)$ where the $p_1 \ldots p_i$ are some set of i parameters to be varied. The spherical symmetry of the potential has been made use of by assuming f depends on $|\rho_1|$ and not on $\vec{\rho}_1$.

Consider

$$(7.21) \quad - \int f(|\rho_1|, p_1 \ldots p_i) \ln f(|\rho_1|, p_1 \ldots p_i) \omega(\rho_1) d^3\rho_1 = I_2$$

$$I_2 = - \int f(|\rho_1|, p_1 \ldots p_i) \ln f(|\rho_1|, p_1 \ldots p_i) \cdot e^{i|\vec{k}|\cdot|\vec{\rho}_1|\cos\theta} \, 2\pi \, d \cos\theta \, |\rho_1|^2 d\rho_1 ,$$

where $\vec{k} = \vec{k}_1 + \vec{k}_2$.

$$I_2 = - 2\pi \int f(|\rho_1|, p_1 \ldots p_i) \ln f(|\rho_1|, p_1 \ldots p_i) |\rho_1|^2 d\rho_1 \cdot (e^{i|k||\rho_1|} - e^{-i|k||\rho_1|}) / ik|\rho_1| .$$

In a free gas case, the plasma mode occurs in the region $|k| << |k_F|$. To simplify the calculation (especially the subsequent integration over $k_1 + k_2$) we shall make the same assumption here. Since the purpose of the calculation is to study the plasma region and since a plasma mode is basically a long range correlation, this should be a valid assumption. If our purpose were to study the correlation energy, short range effects are important and the assumption $|k| << |k_F|$ would no longer be valid. Furthermore, if we are interested in a system such as an atom $|\rho_1|$ is never much larger than 10^{-8} cm. Therefore, we can expand the exponential term and keep only the first nonvanishing term;

$$\frac{e^{i|k||\rho_1|} - e^{-i|k||\rho_1|}}{i|k||\rho_1|} = 2 .$$

Actually, we will presently show that when the specific potential is introduced and all the integrations over ρ_1 performed before making any approximation, we can get the same result without making any assumptions about ρ_1.

With the above approximation we have

$$(7.22)\quad I_1 = -4\pi \int f(|\rho_1|.p_1 \ldots p_i) \ln f(|\rho_1|,p_1 \ldots p_i)\rho_1^2\, d\rho_1 .$$

Consider $-\int u(\rho_1)\omega(\rho_1)f(\rho_1)\, d^3\rho_1$. The first term is

$$(7.23)\quad I_2 = 2\pi i(\omega_1+\omega_2) \int U(|\rho_1|)\, e^{i\,\vec{K}\cdot\vec{\rho}_1} f(|\rho_1|)\, d\cos\theta\, \rho_1^2 d\rho_1$$

and as $k/k_F << 1$,

$$(7.24)\quad I_3 = +4\pi i(\omega_i+\omega_2) \int U(|\rho_1|)\, f(|\rho_1|)\, \rho_1^2\, d\rho_1 .$$

Let

$$(7.25)\quad I_4 = \frac{2\pi i(\omega_1^3+\omega_2^3)\hbar^2}{24m} \int |\nabla U(|\rho_1|)|^2\, \omega(\rho_1)\, f(\rho_1)\, d^3\rho_1$$

$$(7.26)\quad I_4 = \frac{4\pi i(\omega_1^3+\omega_2^3)\hbar^2}{24m} \int |\nabla U(|\rho_1|)|^2\, f(|\rho_1|)\, \rho_1^2\, d\rho_1 .$$

Consider

$$(7.27)\qquad \int f(|\rho_1|\ \omega(\rho_1))\, d^3\rho_1 = I_1\ ;$$

$$(7.28)\qquad I_1 = \int f(|\rho_1| e^{ik\cdot\rho_1})\, d^3\rho_1 .$$

If the potential $U(|\rho_i|)$ were to go to zero, $f(|\rho_1|)$ would be one because at the stationary point $f(x)$ is given by $e^{-u(x)}$.

When $f(|\rho_1|) \to 1$, I_1 appears to be singular when $k \to 0$. Actually there is no singularity after the integration over k is completed. However, it is convenient to subtract out this point and treat it separately i.e.

$$(7.29)\quad I_1 = \int (f(|\rho_1| -1)\, e^{ik\cdot\rho_1}\, d^3\rho_1 + \int e^{ik\cdot\rho_1}\, d^3\rho_1 .$$

Call only the first term I_1. Call the second term I_5.

$$(7.30)\qquad I_5 = (2\pi)^3\, \delta(k)$$

$$(7.31)\qquad I_1 = 4\pi \int (f(|\rho_1|) -1)\rho_1^2\, d\rho_1 .$$

Now suppose the specific potential we are interested in has the form $U(|\rho_1|) = b\, e^{-a|\rho_1|}$. We now need a trial $f(|\rho_1|)$. Referring back to the variational principle we can see that the correct f would be $e^{-u(|\rho_1|)}$. We would like the trial f to be as close to $e^{-u(\rho_1)}$ as possible but easy enough to handle mathematically. A good choice for f, with the specific potential $U(\rho_1)$ mentioned above is

$$f(|\rho_1|) = e^{-Ae^{-\gamma|\rho_1|}} ,$$

where A and γ are the parameters to be varied.

$$I_2 = -\,4\pi \int f(|\rho_1|) \ln f(|\rho_1|)\rho_1^2\, d\rho_1 ,$$

with $f(|\rho_1|) = e^{-Ae^{-\gamma|\rho|}}$.

$$I_2 = 4\pi A \int e^{-A\, e^{-\gamma|\rho_1|}}\, e^{-\gamma|\rho_1|}\, \rho_1^2\, d\rho_1 = 4\pi A \int e^{-Ae^{-\gamma|\rho_1|}}\, e^{-\lambda|\rho_1|}\, \rho_1^2 d\rho_1 \Big|_{\lambda=\gamma}$$

$$= 4\pi A \frac{\partial^2}{\partial\lambda^2} \int_0^\infty e^{-Ae^{-\gamma\rho_1}} e^{-\lambda\rho_1} d\rho_1 \Big|_{\lambda=\gamma} .$$

Let $x = \gamma\rho_1$, $dx = d\rho_1\gamma$.

$$I_2 = \frac{4\pi A}{\gamma} \frac{\partial^2}{\partial\lambda^2} \int_0^A e^{-Ae^{-x}} e^{-\frac{\lambda}{\gamma}x} dx \Big|_{\lambda=\gamma}$$

(7.32) $$I_2 = \frac{4\pi A}{\gamma} \left[\frac{\partial^2}{\partial\lambda^2} [A^{-\frac{\lambda}{\gamma}} \gamma(\tfrac{\lambda}{\gamma}, A)]\right]_{\lambda=\gamma}$$

where $\gamma(\frac{\lambda}{\gamma}, A)$ is the incomplete gamma function. In the same way we get

(7.33) $$I_3 = \frac{4\pi i(\omega_1+\omega_2)b}{\gamma} \left[\frac{\partial^2}{\partial\lambda^2} [A^{-\frac{\lambda}{\gamma}} \gamma(\tfrac{\lambda}{\gamma}, A)]\right]_{\lambda=a}$$

(7.34) $$I_4 = \frac{4\pi i(\omega_1^3+\omega_2^3)\hbar^2 a^2 b^2}{24 m \gamma} \left[\frac{\partial^2}{\partial\lambda^2} [A^{-\frac{\lambda}{\gamma}} \gamma(\tfrac{\lambda}{\gamma}, A)]\right]_{\lambda=2a}$$

(7.35) $$I_1 = \frac{4\pi}{\gamma} \left[\frac{\partial^2}{\partial\lambda^2} [A^{-\frac{\lambda}{\gamma}} G(\tfrac{\lambda}{\gamma}, A)]\right]_{\lambda=0}$$

where $$G(\tfrac{\lambda}{\gamma}, A) = \int_0^A x^{\lambda/\gamma} \frac{e^{-x}-1}{x} dx$$

Using the potential $U(|\rho|) = b\, e^{-a|\rho_1|}$, the ρ_1 integration will now be done before any assumptions about k are made in order to show that no assumptions about the size of ρ_1 are necessary.

We want to evaluate

$$\int e^{-u(\rho_1)} \omega(\rho_1)\, d^3\rho_1$$

where $\omega(\rho_1) = e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{\rho}_1}$

$$u = -i(\omega_1+\omega_2)U(\rho_1) - \frac{i(\omega_1^3+\omega_2^3)\hbar^2}{24m}|\nabla U(\rho_1)|^2$$

$$U(\rho_1) = b\, e^{-a\rho_1}$$

$$|\nabla U(\rho_1)|^2 = a^2b^2\, e^{-2a\rho_1} .$$

Say $= e^{-Ae^{-\gamma\rho_1}}$. Then A and γ are parameters which will be varied. Let $\vec{k} = \vec{k}_1 + \vec{k}_2$.

$$-\int u(\rho_1)\omega(\rho_1)f(\rho_1)\, d^3\rho_1 = -\frac{2\pi(\omega_1+\omega_2)b}{\gamma|k|}\left\{\frac{\partial}{\partial\lambda}(A^{-\lambda/\gamma}\gamma(\frac{\lambda}{\gamma},A)\right\}_{\lambda=a-i|k|}$$

$$+\frac{2\pi(\omega_1+\omega_2)b}{\gamma|k|}\left\{\frac{\partial}{\partial\lambda}[A^{-\lambda/\gamma}\gamma(\frac{\lambda}{\gamma},A)]\right\}_{\lambda=a+i|k|}$$

$$-\frac{2\pi(\omega_1^3+\omega_2^3)\hbar^2a^2b^2}{24\, m\gamma|k|}\left\{\frac{\partial}{\partial\lambda}[A^{-\lambda/\gamma}\gamma(\frac{\lambda}{\gamma},A)]\right\}_{\lambda=2a-i|k|}$$

$$+\frac{2\pi(\omega_1^3+\omega_2^3)\hbar^2a^2b^2}{24\, m\gamma|k|}\left\{\frac{\partial}{\partial\lambda}[A^{-\lambda/\gamma}\gamma(\frac{\lambda}{\gamma},A)]\right\}_{\lambda=2a+i|k|}$$

$$-\int f(|\rho_1|)\ln f(\rho_1)\, e^{ik\cdot\rho_1}\, d^3\rho_1$$

$$= \frac{2\pi iA}{\gamma|k|}\left\{\frac{\partial}{\partial\lambda}[A^{-\lambda/\gamma}\gamma(\frac{\lambda}{\gamma},A)]\right\}_{\lambda=\gamma-i|k|}$$

$$-\frac{2\pi iA}{\gamma|k|}\left\{\frac{\partial}{\partial\lambda}[A^{-\lambda/\gamma}\gamma(\frac{\lambda}{\gamma},A)]\right\}_{\lambda=\gamma+i|k|} .$$

$$\int f(\rho_1)\, e^{ik\cdot\rho_1}\, d^3\rho_1 = \int (f(\rho_1)-1)\, e^{ik\cdot\rho_1}\, d^3\rho_1 + \int e^{ik\cdot\rho_1} d^3\rho_1 .$$

The first term is

$$= + \frac{2\pi i}{\gamma|k|}\left\{\frac{\partial}{\partial\lambda}\,[A^{-\lambda/\gamma}\,G(\frac{\lambda}{\gamma},A)]\right\}_{\lambda=-i|k|}$$

$$- \frac{2\pi i}{\gamma|k|}\left\{\frac{\partial}{\partial\lambda}\,[A^{-\lambda/\gamma}\,G(\frac{\lambda}{\gamma},A)]\right\}_{\lambda=+i|k|}$$

where $\int_0^A x^{\lambda/\gamma}\,(e^{-x}-1)\,\frac{dx}{x}$ is $G(\frac{\lambda}{\gamma},A)$.

The second term is just $(2\pi)^5\delta(k)\cdot I_5$.

In order to be able to perform the integrations over $\vec{k}_1$ and $\vec{k}_2$ it was necessary to make the following approximation. Let

$$\frac{\partial}{\partial\lambda}\,[A^{-\lambda/\gamma}\,G(\frac{\lambda}{\gamma},A)]_{\lambda=\mp i\,k} = g(k)\ .$$

Let

$$\lambda' = \frac{\lambda}{k_F}\ , \qquad \gamma' = \frac{\gamma}{k_F}\ .$$

$$\frac{1}{k_F}\ \frac{\partial}{\partial\lambda'}\ [A^{-\lambda'/\gamma'}\ G(\frac{\lambda'}{\gamma'},A)]_{\lambda'=\mp\frac{ik}{k_F}} = g(\frac{k}{k_F})\ .$$

Assume $|\frac{k}{k_F}| \ll 1$.

$$g(\frac{k}{k_F}) = g(0) + \frac{dg}{d(\frac{k}{k_F})}\bigg|_{\frac{k}{k_F}=0}\cdot\frac{k}{k_F}\ .$$

Call $k/k_F = k'$;

$$\frac{dg}{dk'} = \frac{\partial g}{\partial\lambda'}\ \frac{d\lambda'}{dk'} = \frac{\partial g}{\partial\lambda'}\ (\mp i)\ .$$

The terms with $g(0)$ all cancel.

$$\int (f(\rho_1)-1)\, e^{ik\cdot\rho_1}\, d^3\rho_1 \sim \frac{\pm\, 2\pi i(-i)\cdot 2}{\gamma|k|k_F}\left[\frac{\partial^2}{\partial\lambda'^2} A^{-\frac{\lambda'}{\gamma'}} G(\frac{\lambda'}{\gamma'}, A)\right]_{\lambda'=0}\frac{k}{k_F}$$

$$I_1 = \int (f(\rho_1)-1)\, e^{ik\cdot\rho_1}\, d^3\rho_1 \sim \frac{+4\pi}{\gamma k_F^2}\left[\frac{\partial^2}{\partial\lambda'^2}[A^{-\frac{\lambda'}{\gamma'}} G(\frac{\lambda'}{\gamma'}, A)]\right]_{\lambda'=0}$$

Also,

$$-\int u(\rho_1)\omega(\rho_1)f(\rho_1)\, d^3\rho_1$$

$$\sim \frac{4\pi i(\omega_1+\omega_2)b}{\gamma\, k_F^2}\left\{\frac{\partial^2}{\partial\lambda'^2}[A^{-\frac{\lambda'}{\gamma'}}\gamma(\frac{\lambda'}{\gamma'}, A)]\right\}_{\lambda'=a/k_F}$$

$$+ \frac{4\pi i(\omega_1^3+\omega_2^3)\hbar^2 a^2 b^2}{24m\,\gamma\, k_F^2}\left\{\frac{\partial^2}{\partial\lambda'^2}[A^{-\frac{\lambda'}{\gamma'}}\gamma(\frac{\lambda'}{\gamma'}, A)]\right\}_{\lambda'=2a/k_F}$$

$$= I_3 + I_4 .$$

$$-\int f(\rho_1)\ln f(\rho_1)\, e^{ik\cdot\rho_1}$$

$$\sim \frac{4\pi A}{\gamma\, k_F^2}\left\{\frac{\partial^2}{\partial\lambda'^2}[A^{-\frac{\lambda'}{\gamma'}}\gamma(\frac{\lambda'}{\gamma'}, A)]\right\}_{\lambda'=\gamma/k_F} = I_2 .$$

Since $\lambda' = \frac{\lambda}{k_F}$, $\gamma' = \frac{\gamma}{k_F}$,

$$I_2 = \frac{4A}{\gamma}\left\{\frac{\partial^2}{\partial\lambda^2}[A^{-\lambda/\gamma}\gamma(\frac{\lambda}{\gamma}, A)]\right\}_{\lambda=\gamma} .$$

The same is true for I_1, I_3 and I_4. The agreement with the previously derived I_1, I_2, I_3, I_4 and I_5 is obvious.

4. The Simple Term for the Solution is Reduced to a Two Dimensional Integral.

Consider equation (7.19). The integration over ω_{p_1} was discussed in the last section and the results appeared in the factors I_1, I_2, I_3, I_4, and I_5. Suppose we consider the integration over $\vec{K}_1$ and $\vec{K}_2$ for the terms with I_1, I_2, I_3 and I_4, but not I_5. By using contour integration and decomposition into partial fractions, these integrals were carried out in closed form. Although quite lengthy, this calculation was straightforward and the details will be found in Appendix B.

If we substitute the factors (7.20), B_7 (see Appendix B), (7.22), (7.24), (7.26) and (7.31) into the expression (7.19) and if we neglect for the moment the contribution from the term with I_5, then the last term of $\bar{\mu}(\omega')$ is:

$$(7.36)\quad \bar{\mu}_1(\omega') = \frac{8(2m)^{3/2}q^2\hbar^3 2\pi^3 4^4 8m}{i^{3/2}\ h^6\ \sqrt{\pi}\ \hbar^2}\ \alpha\ \beta \int_{\omega'}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 \Big[\frac{1}{x}$$

$$\cdot\ \frac{(I_1+I_2+I_3+I_4)\ e^{i\omega_2\hbar(\omega-\omega')}\ e^{-iE_F(\omega_1+\omega_2)}}{\omega(\omega_1+\omega_2)^{5/2}}$$

$$\cdot\ -\ \frac{iA_2\hbar^2 x\pi\alpha}{4m}\ e^{-ix\hbar^2\alpha^2/8m}\ \Big(1 - \Phi\Big(\alpha\hbar\sqrt{\frac{-ix}{8m}}\Big)\Big)$$

$$\cdot\ -\ \frac{2C_2 i\hbar^2 x\pi(\alpha+\beta)}{4m}\ e^{-ix\hbar^2(\alpha+\beta)^2/8m}\ \Big(1-\Phi\Big(\hbar(\alpha+\beta)\sqrt{\frac{-ix}{8m}}\Big)\Big)\ -$$

$$- \frac{2iC_3(\alpha+\beta)\hbar^4 x^2}{32m^2} \left[\frac{\sqrt{\pi}}{\hbar \sqrt{\frac{-ix}{8m}}} \right.$$

$$\left. - \pi(\alpha+\beta)\, e^{-ix\hbar^2(\alpha+\beta)^2/8m} \left(1 - \Phi\left(\hbar(\alpha+\beta)\sqrt{\frac{-ix}{8m}}\right)\right)\right]$$

where $x = \frac{\omega_1\omega_2}{\omega_1+\omega_2}$, $A_2 = \frac{-i}{\alpha\, 2^9 \beta^4}$, $C_2 = \frac{i}{\alpha\, 2^{10}\beta^4}$, $C_3 = \frac{i}{\alpha\, 2^{10}\beta^3}$.

The integration over $\vec{k}_1$ and $\vec{k}_2$ for the term with I_5 must now be done.

Remembering that $I_5 = (2\pi)^3\delta(\vec{k}_1+\vec{k}_2)$ we must evaluate:

$$(7.37)\quad (2\pi)^3 \int_{-\infty}^{\infty} d^3k_1 \int_{-\infty}^{\infty} d^3k_2 \frac{\delta(k_1+k_2)\alpha\,\beta\, e^{i|k_1-k_2|\hbar^2\omega_1\omega_2/8m(\omega_1+\omega_2)}}{(k_1^2+\alpha^2)^2\,(k_2^2+\beta^2)^2 k_2^2}$$

$$= \alpha\,\beta(2\pi)^3 \int_{-\infty}^{\infty} \frac{d^3k_1\; e^{i|k_1|^2\hbar^2\omega_1\omega_2/2m(\omega_1+\omega_2)}}{(k_1^2+\alpha^2)^2\,(k_1^2+\beta^2)k_1^2}$$

$$= 32\pi^4\alpha\,\beta \int_0^{\infty} d|k_1| \frac{e^{ik_1^2\hbar^2\omega_1\omega_2/2m(\omega_1+\omega_2)}}{(k_1^2+\alpha^2)^2\,(k_1^2+\beta^2)^2}$$

Making use again of the method of partial fractions:

$$\frac{1}{(k_1^2+\alpha^2)^2(k_1^2+\beta^2)^2} = \frac{E_2}{(k_1^2+\alpha^2)^2} + \frac{E_1}{(k_1^2+\alpha^2)} + \frac{F_2}{(k_1^2+\beta^2)^2} + \frac{F_1}{(k_1^2+\beta^2)}$$

$$E_2 = \frac{1}{(\beta^2-\alpha^2)^2},\quad E_1 = \frac{-2}{(\beta^2-\alpha^2)^3},\quad F_2 = \frac{1}{(\alpha^2-\beta^2)^2},\quad F_1 = \frac{-2}{(\alpha^2-\beta^2)^3}$$

The integration was then completed by using standard integral tables.

We substitute the integrated form into the expression (7.19) to get the correction to $\bar{\mu}(\omega')$ due to the term with I_5. This correction is:

$$(7.38)\quad \frac{q^2 8(2m)^{3/2}\hbar^3 \alpha\,\beta\, 32\pi^4}{i^{3/2}\, h^6 \sqrt{\pi}} \int_{\omega'}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2$$

$$\cdot \frac{e^{i\omega_2\omega\hbar - i\omega'\hbar\omega_2 - iE_F(\omega_1+\omega_2)}}{\omega(\omega_1+\omega_2)^{5/2}}$$

$$\begin{aligned}
\cdot \Bigg\{ & \frac{1}{(\beta^2-\alpha^2)^2}\ \frac{i\hbar^2 x}{2m}\ [1 - \underline{\Phi}\ (\alpha\hbar \sqrt{\frac{-ix}{2m}}\ )]\ \frac{\pi}{2\alpha}\ e^{-i\alpha^2\hbar^2 x/2m} \\
& - \frac{1}{(\beta^2-\alpha^2)^2}\ \frac{i\hbar^2 x}{\alpha^2 2m}\ \frac{\sqrt{\pi}\ \sqrt{2m}}{2\hbar\sqrt{-ix}} \\
& + \frac{1}{\alpha^2(\beta^2-\alpha^2)^2}[1 - \underline{\Phi}\ (\alpha\hbar \sqrt{\frac{-ix}{2m}}\ )]\ \frac{\pi}{2\alpha}\ e^{-i\alpha^2\hbar^2 x/2m} \\
& + \frac{1}{(\alpha^2-\beta^2)^2}\ \frac{i\hbar^2 x}{2m}\ [1 - \underline{\Phi}(\beta\hbar \sqrt{\frac{-ix}{2m}}\ )]\ \frac{\pi}{2\beta}\ e^{-i\beta^2\hbar^2 x/2m} \\
& - \frac{i\hbar^2}{(\alpha^2-\beta^2)^2}\ \frac{x}{\beta^2\ 2m}\ \frac{\sqrt{\pi}}{2\hbar}\ \frac{\sqrt{2m}}{\sqrt{-ix}} \\
& + \frac{1}{(\alpha^2-\beta^2)^2\beta^2}\ [1-\underline{\Phi}(\beta\hbar \sqrt{\frac{-ix}{2m}}\ )]\frac{\pi}{2\beta}\ e^{-i\beta^2\hbar^2 x/2m} \\
& - \frac{2}{(\beta^2-\alpha^2)^3}\ \frac{\pi}{2\alpha}[1-\underline{\Phi}(\alpha\hbar \sqrt{\frac{-ix}{2m}}\ )]e^{-i\hbar^2\alpha^2 x/2m} \\
& - \frac{2}{(\alpha^2-\beta^2)^3}\ \frac{\pi}{2\beta}\ [1 - \underline{\Phi}(\beta\ \hbar \sqrt{\frac{-ix}{2m}}\ )]\ e^{-i\hbar^2\beta^2 x/2m} \Bigg\}.
\end{aligned}$$

5. The Complete General Solution Expressed as a Two Dimensional Integral.

If we refer back to equations (7.9) and (7.16), we see that we have calculated only part of the contribution to $\bar{\mu}(\omega')$. However, as was stated before, the additional terms are so similar to the ones we have calculated that we can evaluate their contributions without redoing the calculation for each term. Consider first all the contributions to the direct term for $\bar{V}$. We notice that the integrations in r, r_1, r_2, p_1 and p_2 are all the same.

The contribution to $\bar{\mu}(\omega')$ that was calculated corresponds to the last term in $\bar{V}$. This term contains the following integral with respect to ω:

$$\int_{\omega'}^{\infty} \frac{d\omega\, e^{i\omega_2\hbar\omega}}{\omega} \quad \text{and this equals} \quad -E_i(i\omega_2\hbar\,\omega')$$

where E_i ia the exponential integral.

Consider the second term in $\bar{V}(\bar{r}_2, \bar{r}_1, \omega')$. This term contains the factor: $\int_{-\infty}^{\omega'} e^{-i\omega_1\omega\hbar}\, d\omega/\omega$ which equals

$$\fint_{-\infty}^{\omega'} (e^{-i\omega_1\omega\hbar}\, d\omega/\omega) - i\pi \int \delta(\omega)\, d\omega\, e^{-i\omega_1\omega\hbar}$$

where $\fint$ stands for the principal part, and

$$\fint_{-\infty}^{\omega'} e^{-i\omega_1\omega\hbar}/\omega = -E_i(-i\omega'\hbar\,\omega_1) .$$

Consider first the contribution from the principal part.

If we replace ω' by $-\omega'$, we see that this term looks exactly like the third and last term except for a minus sign and the fact that the roles of ω_1 and ω_2 are interchanged. Since the paths of integration for ω_1 and ω_2 are the same, we can interchange their names without changing the value of the integral. Hence, this term is the same as the last term with the following changes: (1) multiply by -1, (2) let $\omega' \rightarrow -\omega'$.

By the same reasoning, the term with $\delta(\omega)$ is the same as the last term with the following changes: (1) multiply by $i\pi$, (2), let $\omega' \rightarrow -\omega'$, (3) omit the exponential integral factor.

In the first term of $\overline{V}$, $(t-t')/\hbar$ plays the role of ω_2. We get the same contribution to $\bar{\mu}_1(\omega')$ as from the last term with $-E_i[i\hbar\omega_2\omega']$ replaced by $2\pi i\theta(-\hbar\omega_2)$.

Now consider the exchange term, the second term in (5.4). Again the calculations are very similar and the results can be obtained by simple changes in the direct term.

In the first term of $\overline{V}$ exchange, $(t'-t)/\hbar$ plays the role of ω_2. This term is exactly the same as the first term of $\overline{V}$ direct with $\omega' \rightarrow -\omega'$.

The results for the other terms are such that all the terms involving the exponential integral function cancel those of the direct term and the part arising from the point contribution $-i\delta(\omega)$ is exactly the same.

Let $I(\omega', \omega_1, \omega_2)$ be the sum of the integrands of the expressions (7.36) and (7.38). Denote the sum of the contributions to $\bar{\mu}(\omega')$ from all the terms by $\bar{\mu}(\omega')_{total}$. Then

$$(7.39)\quad \bar{\mu}(\omega')_{total} = \int d\omega_1 \int d\omega_2 \, [2\pi i \, I(-\omega', \omega_1 \; \omega_2)$$

$$- 2\pi i \, I(\omega', \omega_1 \; \omega_2)\theta(-\hbar\omega_2) - 2\pi i \, I(-\omega', \omega_1, \omega_2)\theta(-\hbar\omega_2)].$$

Note that the integration over $d\omega$ has been accounted for in this expression. From now on the subscript total will be omitted and $\bar{\mu}(\omega')$ will be understood to be the total value.

6. This Method Applied to a Uniform Electron Gas - The Solution for a Uniform Electron Gas Expressed as a Two Dimensional Integral.

It is worthwhile at this point to repeat the calculation of $\bar{\mu}(\omega')$ for the free electron gas case using the same techniques and orders of operations as for the inhomogeneous case. Of course, this is a roundabout and clumsy way to handle the free electron gas case. However, there are two important purposes in doing this. First, it is a convenient way of checking $\bar{\mu}(\omega', \omega_1 \; \omega_2)$ for the inhomogeneous case since this must reduce to $\bar{\mu}(\omega', \omega_1 \; \omega_2)$ as the potential goes to zero, or to a constant. Second, since the integrations in ω_1 and ω_2 are difficult, we can be guided in the method by performing them in the free gas case where we already know the answer.

Refer now to the expression for (5.6) for $\mu(\omega')$. In the free gas case we already know the values for $\chi(\vec{r})$ and $\phi(\vec{r})$.

$$\chi(\vec{r}\,) = e^{i\vec{k}\cdot\vec{r}\,'}$$

$$\phi(\vec{r}\,') = e^{-i\vec{k}\cdot\vec{r}\,'}$$

Also, the expression (7.2) for $\rho(\vec{x},\vec{x}\,')$ with $U(x)$ and $\nabla U(x)$ both equal to zero is the exact density operator for the free gas.

We repeat all the steps as before.

The expression (7.16) is replaced by

$$(7.40)\quad \mu(\omega') = \bar{\mu}(\omega') = \int_{-\infty}^{\infty} d^3p_1\, d^3p_2\, d\omega_1\, d\omega_2\, d^3\rho_1\, d^3\rho_2\, d^3\rho_3 \int_{\omega'}^{\infty} d\omega$$

$$\cdot\ \frac{-2q^2}{ih^6\pi^2}\left[\frac{e^{i\omega\omega_2\hbar - i\omega'\hbar\omega_2}}{\omega(\omega_1+\omega_2)}\, \frac{1}{|\rho_2|}\, e^{i\vec{k}\cdot(\vec{\rho}_1+\vec{\rho}_3)}\, e^{-i\vec{k}\cdot(\rho_1-\rho_3-\rho_2)}\right.$$

$$\left.\cdot\ e^{ip_1\cdot 2\rho_3/\hbar}\, e^{-ip_2\cdot 2\rho_3/\hbar}\, e^{-i\omega_1(E_F-p_1^2/2m)-i\omega_2(E_F-p_2^2/2m)}\right]$$

Notice that this can be obtained from the general expression simply by the following substitutions:

$$\frac{\phi(k_1)}{2\pi^3} = \frac{\psi(k_2)}{(2\pi)^3} = 1$$

$$\vec{k} = \vec{k}_1 = -\vec{k}_2$$

$$U(\rho_1) = 0$$

$$\nabla U(\rho_1) = 0$$

Continuing the calculation we find for $\mu_{free}(\omega')$:

$$(7.41)\quad \frac{q^2 8(2m)^{3/2}\hbar^3\pi^4}{i^{3/2}h^6\sqrt{\pi}\,k^2}\int d\omega_1\,d\omega_2\,\left[\frac{e^{\frac{ik^2\hbar^2\omega_1\omega_2}{2m(\omega_1+\omega_2)}}\,e^{-i(\omega_1+\omega_2)E_F}}{(\omega_1+\omega_2)^{5/2}}\right.$$

$$\cdot\,[2\pi i\,e^{i\omega'\hbar\omega 2}-2\pi i\,e^{-i\omega'\hbar\omega_2}\,\theta(-\hbar\omega_2)$$

$$-\,2\pi i\,e^{i\omega'\hbar\omega_2}\,\theta(-\,\omega_2)]\,.$$

7. The Limit of the General Solution when the External Potential Goes to Zero.

We now want to show that the general expression (7.39) for $\bar{\mu}(\omega')$ reduces to the free case, expression (7.41), when the potential goes to zero.

Referring back to the variational principle (7.20) we see that $u(\rho_1) = 0$ when the potential is identically zero. When $u(\rho_1) = 0$, the $f(|\rho_1|) \rightarrow 1$. The terms I_1, I_2, I_3 and I_4 must all be zero and we are left with only the term with I_5.

We have evaluated explicitly I_1, I_2, I_3 and I_4 for the specific potential $U(|\rho_1|) = b\,e^{-a|\rho_1^2|}$. Suppose $b \equiv 0$. We must show that I_1, I_2, I_3 and I_4 are in fact equal to zero. Since I_3 is proportianal to b, and I_4 to b^2, these two terms are obviously zero when b is zero. Consider the trial function $f(|\rho_1|)$. As was stated previously the correct f would be $e^{-u(|\rho_1|)}$, which should now be 1.

We had assumed that $f(|r_1|) = -A e^{-\gamma|r_1|}$. We see then that when the potential goes to zero, A will go to zero or γ must go to infinity. With either of these conditions, I_1, I_2, I_3 and I_4 all equal zero identically.

To complete the argument we must show that the I_5 term, which appears in expression (7.38), reduces to the free case.

In the general case we chose trial eigenfunctions for the integral equation, i.e.

$$\chi(r) = e^{-\alpha r}$$

$$\Phi(r') = e^{-\beta r'} .$$

In the free case we know that we have

$$\chi(r) = e^{ik\cdot r}$$

$$\Phi(r') = e^{-ik\cdot r'}$$

When the potential goes to zero χ and Φ must approach the free gas functions. Because of the spherical symmetry of the trial functions, they can equal the free functions only when k equals 0. In this case both α and β equal 0. In addition, they must go to zero such that $\alpha = -\beta$. If we take the limit of expression (7.38) as $\alpha \rightarrow -\beta$, and then as $\alpha \rightarrow 0$, we can show that (7.38) becomes equal to the free case for k equal to zero. If we want to consider k very small but not actually zero we really should not compare (7.38) with (7.41). Instead of (7.41) we should look at the s state free gas case, i.e. the eigenfunctions χ and Φ should be the s state components of plane waves and not just plane waves. However, if we let $\alpha \to ik$ and $\beta \to -ik$ as α and β become small we find that expression (7.38) reduces to (7.41) without having to set k equal to zero.

If we take the limit of (7.38) as $\alpha \to -\beta$ and then as $\alpha \to 0$ noting that $\lim\limits_{x \to 0} \Phi(x) \to 0$, we find that only the last two terms of (7.38) contribute as all the other terms cancel. These last two terms are:

$$(7.42)\quad \bar{\mu}(\omega', \omega_1\ \omega_2) = \frac{q^2 8(2m)^{3/2} \hbar^3 \alpha\ \beta\ 32\pi^4}{i^{3/2}\ h^6\ \sqrt{\pi}} \cdot \frac{e^{-iE_F(\omega_1+\omega_2)}}{(\omega_1+\omega_2)^{5/2}}$$

$$\cdot (2\pi i\ e^{i\omega'\hbar\omega_2} - 2\pi i e^{-i\omega'\hbar\omega_2})\theta(-\hbar\omega_2) - 2\pi i e^{i\omega'\hbar\omega_2}\ \theta(-\hbar\omega_2))$$

$$\cdot [\frac{2}{(\beta^2-\alpha^2)^3} \frac{\pi}{2\alpha} [1-\Phi(\alpha\hbar\sqrt{\frac{-ix}{2m}})]e^{-i\hbar^2\alpha^2 x/2m}$$

$$- \frac{2}{(\alpha^2-\beta^2)^3} \frac{\pi}{2\beta} [1-\Phi(\beta\hbar\sqrt{\frac{-ix}{2m}})]e^{-i\hbar^2\beta^2 x/2m}].$$

Since it is $\mu(\omega')$ we are comparing and not $\bar{\mu}(\omega')$ we must multiply the whole expression by the normalization factor $(\alpha+\beta)^3/8\pi$. Also:

$$(\beta^2 - \alpha^2) = (\beta+\alpha)(\beta-\alpha)$$

So

$$(7.43)\quad \lim_{U(|\rho_1|)\to 0} \mu(\omega') \to \frac{q^2 8(2m)^{3/2}\hbar^3\, 4\pi^4}{i^{3/2}\, h^6\, \sqrt{\pi}}\; \frac{\alpha\beta(\alpha+\beta)^3}{3\pi}$$

$$\times\,(\text{terms in } \omega_1, \omega_2, \omega') \times [\frac{-2}{(\beta+\alpha)^3(\beta-\alpha)^3}\,\frac{\pi}{2\alpha}[1-\Phi(\alpha\hbar\sqrt{\frac{-ix}{2m}}\,)]$$

$$\times\, e^{i\hbar^2\alpha^2 x/2m} + \frac{2}{(\beta+\alpha)^3(\beta-\alpha)^3}\,\frac{\pi}{2\beta}\,[1-\Phi(\beta\hbar\sqrt{\frac{-ix}{2m}}\,)]e^{-i\hbar^2\beta^2/2m}].$$

Cancelling the $(\alpha+\beta)^3$ terms we have

$$(7.44)\quad \lim_{U|\rho_1|\to 0} \mu(\omega') \to \frac{q^2 8(2m)^{3/2}\hbar^3\, 4\pi^4}{i^{3/2}\, h^6\, \sqrt{\pi}}\, \alpha\beta \int d\omega_1\, d\omega_2\, \frac{e^{-i(\omega_1+\omega_2)E_F}}{(\omega_1+\omega_2)^{5/2}}$$

$$\cdot[2\pi i\, e^{i\omega'\hbar\omega_2} - 2\pi i\, e^{-i\omega'\hbar\omega_2}\,\theta(-\hbar\omega_2) - 2\pi i e^{i\omega'\hbar\omega_2}\,\theta(-\hbar\omega_2)]$$

$$\cdot[-\frac{1}{(\beta-\alpha)^3\alpha}\,[1-\Phi(\alpha\hbar\sqrt{\frac{-ix}{2m}}\,)]\, e^{-i\hbar^2\alpha^2 x/2m}$$

$$+\frac{1}{(\beta-\alpha)^3\beta}\,[1-\Phi(\beta\hbar\sqrt{\frac{-ix}{2m}}\,)]\, e^{-i\hbar^2\beta^2 x/2m}].$$

Now let $\beta \to -\alpha$.

$$\lim_{\beta\to -\alpha} \alpha\beta\,(-\frac{1}{(\beta-\alpha)^3\alpha} + \frac{1}{(\beta-\alpha)^3\beta}) = -\frac{1}{4\alpha^2}.$$

Also, as $\alpha,\beta \to 0$, since $\Phi(x)_{x\to 0} = \frac{2}{\sqrt{\pi}}\cdot x$,

the error functions cancel.

Letting $\alpha \to ik$,

$$-\frac{1}{4\alpha^2} = \frac{1}{4k^2} \quad\text{and}\quad e^{-i\hbar^2\alpha^2 x/2m} = e^{-i\hbar^2\beta^2 x/2m} = e^{i\hbar^2 k^2 x/2m}.$$

Therefore

$$(7.45) \quad \lim_{\text{potential}\to 0} \mu(\omega') = \frac{q^2 8(2m)^{3/2}\, \hbar^3 \pi^4}{i^{3/2}\, h^6\, \sqrt{\pi}}$$

$$\cdot \int \frac{d\omega_1\, d\omega_2\, e^{-i(\omega_1+\omega_2)E_F}}{(\omega_1+\omega_2)^{5/2}}\, e^{i\hbar^2 k^2 x/2m}$$

$$\cdot\, [2\pi i\, e^{i\omega'\hbar\omega_2} - 2\pi i\, e^{-i\omega'\hbar\omega_2}\, \theta(-\hbar\omega_2) - 2\pi i\, e^{i\omega'\hbar\omega_2}\, \theta(-\hbar\omega_2)]$$

where $x = \omega_1\omega_2/(\omega_1+\omega_2)$.

We see that this equals $\mu(\omega')_{\text{free}}$!

8a. The Remaining Integrations for the Uniform Gas Are Approximated by the Method of Steepest Descent.

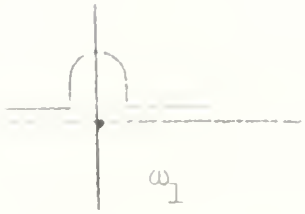
In the general case, the ω_1 and ω_2 integrations could not be done analytically in closed form and an approximation method had to be developed. For this purpose, we studied these integrations for the free case. Although the free gas case can be calculated exactly by other methods, we wanted to use the same methods here as we would use in the more general case. Since we knew the answer, the validity of any approximations could then be checked. It should be remarked here that (7.41) $\mu_{\text{free}}(\omega')$ is exact. Therefore the only approximation made in the free gas case is what will be involved in the ω_1 and ω_2 integrations.

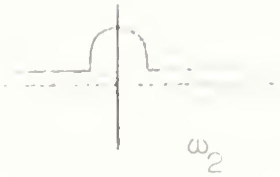
To facilitate the calculation, we made the following transformation:

$$\omega_2 = \omega_2$$

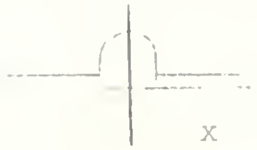
$$\frac{\omega_1\omega_2}{\omega_1+\omega_2} = x \; , \quad \omega_1 = \frac{\omega_2 x}{\omega_2 - x} \; . \quad \text{Jacobian} = \frac{\omega_2^2}{(\omega_2 - x)^2} \; , \quad \omega_1 + \omega_2 = \frac{\omega_2^2}{\omega_2 - x}$$

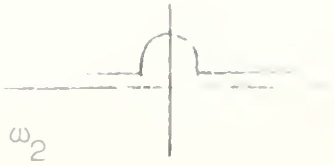
It is important to remember that the paths for ω_1 and ω_2 were





The new paths will be





With this transformation the expression (7.41) becomes

$$(7.46) \quad \mu_{\text{free}}(\omega') = \frac{q^2 8 (2m)^{3/2}}{i^{3/2}\, \hbar^6} \frac{\hbar^3 \pi^4}{\sqrt{\pi}\, k^2}$$

$$\cdot \int dx \int d\omega_2 \, \frac{(\omega_2 - x)^{1/2}}{\omega_2^3} \, e^{-iE_F\left(\frac{\omega_2^2}{\omega_2 - x}\right)} \, e^{i \frac{k^2\hbar^2 x}{2m}}$$

$$\cdot \left[2\pi i \, e^{i\omega'\hbar\omega_2} - 2\pi i \, e^{-i\omega'\hbar\omega_2} \theta(-\hbar\omega_2) - 2\pi i \, e^{i\omega'\hbar\omega_2} \theta(-\hbar\omega_2) \right]$$

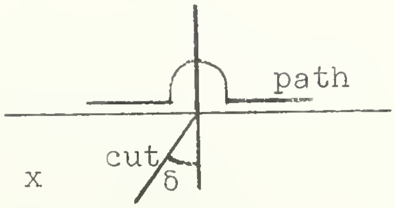
Consider now the integral

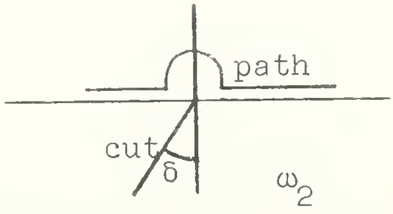
$$(7.47) \quad \int dx \int d\omega_2 \, \frac{(\omega_2 - x)^{1/2}}{\omega_2^3} \, e^{-iE_F\left(\frac{\omega_2^2}{\omega_2 - x} + n\omega_2\right)} \, e^{\frac{ik^2\hbar^2 x}{2m}} \, \theta(-\hbar\omega_2)$$

where $n = \frac{\hbar\omega'}{E_F}$. (n is not necessarily an integer.)

This corresponds to the middle term of the factor in brackets in (7.46). The other terms are so similar that they can be evaluated by the same methods as this one.

The factor $(\omega_2-x)^{1/2}$ necessitates a branch cut. The paths for x and ω_2 should not cross any branch cuts. Therefore, we must remember during the calculation to choose the branch cuts in the following way:





where we leave the angle δ undefined for the present.

We will now try to approximate the x and ω_2 integrations by the method of steepest descent through the saddle point keeping only leading terms.

Making use of standard techniques the method of steepest descent yields the following formulas:

$$(7.48)\quad \int e^{zh(t)}\,dt = e^{zh(t_0)}\sqrt{\frac{\pi a_0^2}{\tau}}\sum_{n=0}^{\infty}\left(\frac{a_{2n}}{a_0}\right)\frac{\Gamma(n+\frac{1}{2})}{\Gamma(\frac{1}{2})}\left(\frac{1}{z}\right)^n$$

where $a_n = \frac{1}{n!}\frac{d^n}{dt^n}\left[\frac{t-t_0}{g(t)}\right]^{n+1}$, $g(t) = \sqrt{h(t_0) - h(t)}$, t_0 is the saddle point.

Using

$$\left(\frac{h(t_0)-h(t)}{(t-t_0)^2}\right) = \sum_p A_p(t-t_0)^p$$

where the A_p are obtained from a Taylor expansion of h(t), we have

$$a_n = \frac{1}{n!}\left\{\frac{d^n}{dx^n}\left[\sum_p A_p x^p\right]^{-\frac{1}{2}n-\frac{1}{2}}\right\}_{x=0}$$

When evaluated explicitly, the first few a_n are:

$$a_0 = \frac{1}{\sqrt{A_0}}\,, \qquad a_1 = -\frac{A_1}{A_0^2}\,,$$

$$\frac{a_2}{a_0} = \frac{15}{8}A_1^2A_0^{-3} - \frac{3}{2}A_2A_0^{-1/2}$$

(7.49)

$$\frac{a_4}{a_0} = \frac{5\cdot7\cdot9\cdot11}{2^7\cdot3}A_1^4A_0^{-4} - \frac{5\cdot7\cdot9\cdot A_0^{-5}A_1^2A_2}{24}$$

$$+\frac{5\cdot7}{2^3}A_0^{-4}(A_2^2 + 2A_1A_3) - \frac{5}{2}A_0^{-3}A_4\,.$$

This method is now applied to equation (7.47). We must bear in mind that the path of integration is now the one of steepest descent and not the original path. For this to be valid the deformation of the contour should not change the value of the integral. If this is not the case, then it is necessary to add corrections to the path of steepest descent. This point will be discussed more clearly and in more detail when we know what the steepest path is.

In equation (7.47) we have $\theta(-\hbar\omega_2)$ where θ is the step function. Since the step function is defined only on the real axis, before proceeding, we must by analytic continuation define a function which is defined throughout the complex plane and which reduces to the step function on the real axis. Such a function is:

$$\theta(z) = \frac{1}{\pi} \arg(-z), \text{ so}$$

(7.50)

$$\theta(-\hbar\omega_2) = \frac{1}{\pi} \arg(\hbar\omega_2) = \frac{1}{\pi} \operatorname{Imag}(\operatorname{Log}(\hbar\omega_2)) .$$

For this function to be uniquely defined, we must make a branch cut. This is done in the manner already described. Since this function is not analytic, the choice of the continued function is not unique. However, we have not made use of any specific representation for the step function so far in the problem, i.e., we have used only the properties on the real axis and so any representation will serve us now.

We must now find the saddle point for equation (7.47). This involves finding the saddle point in a four dimensional space whereas standard methods usually treat only a two dimensional space. Therefore, this point will be discussed in detail.

One method of finding the saddle point in four dimensions is to treat two dimensions at a time in a self-consistent way. This was tried and led to very bad agreement with the exact answer. It is obviously more correct to take the four dimensions at once, but it is also more difficult. However, we worked it out in the following way: We rewrite equation (7.47) as

$$(7.51) \int dx \int d\omega_2 \, e^{\left[-iE_F\left(\frac{\omega_2^2}{\omega_2 - x} + n\omega_2\right) + i\frac{k^2\hbar^2 x}{2m} + \frac{1}{2}\ln(\omega_2 - x) - 3\ln\omega_2\right]} \cdot \theta(-\hbar\omega_2).$$

We know that the plasma frequency is given in the limit as $k \rightarrow 0$. Therefore it is correct to assume that

$$\frac{k^2\hbar^2}{E_F\,2m} << 1 .$$

When we apply these same methods to the general case, we will use a similar condition:

$$\text{(7.52a)} \qquad \frac{\left|\dfrac{\alpha^2\hbar^2 x_0}{2m}\right|}{\left|E_F\left(\dfrac{\omega_{2_0}^2}{\omega_{2_0}-x_0}+n\omega_{2_0}\right)\right|} << 1$$

and

$$\text{(7.52b)} \qquad \frac{\left|(\alpha+\beta)^2\hbar^2 x_0\right|}{\left|E_F\left(\dfrac{\omega_{2_0}^2}{\omega_{2_0}-x_0}+n\omega_{2_0}\right)\right|} << 1 .$$

where x_0 and ω_{2_0} are the saddle points.

Aside from the similarity to the free gas case we have no a priori method of knowing that these assumptions are correct. However, at the end, when the numerical values are known, these assumptions turn out to be very, very good. They are therefore justified by self-consistency.

The saddle point is found by taking the derivatives of the exponent with respect to x and to ω_2, setting these equal to zero, and solving the resulting two simultaneous equations. For maximum accuracy, we should include the whole integrand in the exponent, for example, writing $\theta(-\hbar\omega_2)$ as $e^{\ln\theta(-\hbar\omega_2)}$. The inclusion of all the factors in the exponent was too cumbersome to handle. However, with the exception of the $\theta(-\hbar\omega_2)$, all the other terms were included. The error introduced by not putting $\theta(-\hbar\omega_2)$ into the exponent is discussed together with the error introduced by keeping only the leading terms in Section 8b of this chapter.

Referring to the exponent as $E(\omega_2,x)$ we have from equation (7.51)

$$(7.53)\quad E(\omega_2,x) = -iE_F\left(\omega_2+x+\frac{x^2}{\omega_2-x}+n\omega_2\right)+\frac{1}{2}\ln(\omega_2-x)-3\ln\omega_2$$

for $\frac{k^2\hbar^2}{E_F 2m} << 1$, and where we have written $\frac{\omega_2^2}{\omega_2-x}$ as $\omega_2+x+\frac{x^2}{\omega_2-x}$

$$0 = \frac{\partial E}{\partial\omega_2}+\frac{\partial E}{\partial x} : \quad -i\,E_F\left(2+\frac{2x}{\omega_2-x}+n\right) = \frac{3}{\omega_2}$$

$$0 = \frac{\partial E}{\partial x} : \quad -i\,E_F\left(1+\frac{2x}{\omega_2-x}+\frac{x^2}{(\omega_2-x)^2}\right) = \frac{1}{2(\omega_2-x)}$$

Letting $\lambda = \frac{x}{\omega_2-x}$ we have

$$-i\,E_F\,(2+2\lambda+n) = \frac{3}{\omega_2}$$

$$-i\,E_F\,(1+\lambda) = \frac{1}{2\omega_2}$$

These two equations have the solution

$$(7.54)\qquad \lambda = \frac{n}{4}-1\,,\quad \omega_{2_0} = \frac{2}{-iE_F n}\,,\quad x_0 = \frac{\omega_{2_0}\lambda}{1+\lambda} = \frac{8(\frac{n}{4}-1)}{-iE_F n^2}$$

Using this saddle point, the method of steepest descent is used separately for ω_2 and x in order to calculate the coefficients in the expansion. Also, in the x part, the above x_0 will be improved by including the contribution from $e^{ik2h^2x/2m}$ which was neglected in the above derivation of x_0.

From equation (7.51), the terms in the exponent involving only ω_2 are:

$$h(\omega_2) = -i\ E_F(\omega_2 + x + \frac{x^2}{\omega_2 - x} + n\omega_2) + \frac{1}{2}\ln(\omega_2 - x) - 3\ln\omega_2 .$$

We evaluate $\frac{\partial^2}{\partial\omega_2^2} h(\omega_2)$ substituting the above values for x_0 and ω_{2_0} to get $h''(\omega_{2_0})$. Using

$$A_0 = -\frac{1}{2} h''(\omega_2^0), \qquad a_0 = \frac{1}{\sqrt{A_0}} ,$$

we get

$$a_{0_{\omega_2}} = \frac{16}{E_F n\sqrt{n^2-18n+128}} ,$$

the leading term for

$$(7.55) \qquad \int e^{h(\omega_2)}\, d\omega_2 = e^{h(\omega_{2_0})} \sqrt{\pi}\, a_{0_{\omega_2}} .$$

As was already mentioned we want to improve x_0 to include the effect of the k^2 term. Therefore we do not use x_0 and ω_{2_0} when evaluating $h(\omega_{2_0})$. Instead, we do the following. We had

$$\lambda = \frac{x}{\omega_2 - x} , \qquad x = \frac{\omega_2\lambda}{1+\lambda} ,$$

so

$$\omega_2 - x = \frac{\omega_2}{1+\lambda} \;, \qquad \omega_2 = \frac{x(1+\lambda)}{\lambda} \;.$$

λ was calculated to be $\frac{n}{4}-1$, and using the value of λ, we substitute into $h(\omega_2)$

$$\omega_2 = x\left(\frac{n}{n-4}\right) \;, \qquad \omega_2 - x = \frac{x}{\frac{n}{4}-1} \;.$$

We find for the leading term:

$$\sqrt{\pi}\; a_{0\omega_2} \frac{\sqrt{x}\;(n-4)^3}{\sqrt{\frac{n}{4}-1}\; x^3 n^3}\; e^{-iE_F N x + \frac{ik^2\hbar^2 x}{2m}}\; \theta\left(-x\hbar\,\frac{n}{n-4}\right) \tag{7.56}$$

where $N = \frac{5}{4}\,\frac{n^2}{n-4}$.

As before, taking all the x terms into the exponent except for the factor $\theta(-x\hbar\,\frac{n}{n-4})$, the exponent is

$$h(x) = -\,i\,g\,x - \frac{5}{2}\log x \;, \qquad g = E_F N - \frac{k^2\hbar^2}{2m} \;, \tag{7.57}$$

$$h'(x) = -\,ig - \frac{5}{2x} \;, \quad h'(x_0) = 0, \quad x_0 = \frac{5i}{2g} \;.$$

If we let $k \to 0$ then

$$x_0 \to \frac{5i}{2E_F N} = \frac{5i}{2E_F\,\frac{5}{4}\,\frac{n^2}{n-4}} = \frac{2i(n-4)}{E_F(n^2)} \tag{7.58}$$

which is the same as the first x_0 we found. Similarly

$$\begin{aligned} \omega_{2_0} &= x_0\left(\frac{n}{n-4}\right) \quad \text{and} \\ \omega_{2_0} &\to \frac{n}{n-4}\,\frac{5i}{2E_F\,\frac{5}{4}\,\frac{n^2}{n-4}} = \frac{2i}{E_F n} \qquad \text{as } k \to 0, \end{aligned} \tag{7.59}$$

which is the same as the first ω_{2_0}, i.e. expression (7.54).

Therefore, we have now corrected x_0 and ω_2 to include the effect of the k^2 term.

The leading term for the x integration is

$$(7.60) \qquad \int \Phi(x)\, e^{h(x)}\, dx = \Phi(x_0)\, e^{h(x_0)} \sqrt{\pi}\, a_{0_x} ,$$

where $\qquad a_0 = \frac{1}{\sqrt{A_x}}, \quad A_x = -\frac{1}{2} h''(x_0)$ and $a_0 = \frac{\sqrt{5}}{g}$.

The leading term for equation (7.47) becomes:

$$(7.61) \qquad \frac{\pi\, a_{0_{\omega_2}}\, a_{0_x} (n-4)^2}{\sqrt{\frac{n}{4}-1}\; n^2 \left(\frac{5i}{2g}\right)^{5/2}}\; e^{5/2}\; \theta\!\left(-\frac{\hbar n}{n-4}\, \frac{5i}{2g}\right) .$$

Referring back to the expression (7.45) for $\mu(\omega')_{\text{free}}$, we note that the last term is the same as this term with $n \rightarrow -n$. The first term is also the same if $n \rightarrow -n$ and if $\theta(-\hbar\omega_2) \equiv 1$.

Therefore the leading term for $\mu(\omega')_{\text{free}}$ is:

$$(7.62) \quad \mu(\omega')_{\text{free}} = \frac{q^2\, 8(2m)^{3/2}\, \hbar^3 \pi^5}{i^{3/2}\, h^6 \sqrt{\pi}\, k^2}\; \frac{e^{5/2}\, 2^{5/2}}{25}$$

$$\cdot \left[2\pi i\, K_2\, g_2^{3/2} - 2\pi i K_1\, g_1^{3/2}\, \theta\!\left(-\frac{\hbar n}{n-4}\, \frac{5i}{2g_1}\right) - 2\pi i\, K_2\, g_2^{3/2}\right.$$

$$\left. \cdot\, \theta\!\left(-\frac{\hbar n}{n-4}\, \frac{5i}{2g_2}\right)\right] ,$$

where $\qquad g_1 = E_F N_1 - \frac{k^2\hbar^2}{2m}, \qquad g_2 = E_F N_2 - \frac{k^2\hbar^2}{2m}$,

$$N_1 = \frac{5}{4}\left(\frac{n^2}{n-4}\right), \qquad N_2 = -\frac{5}{4}\left(\frac{n^2}{n+4}\right),$$

$$K_1 = \frac{2^5 (n-4)^{5/2}}{E_F n^4 \sqrt{n^2-16n+128}}, \qquad K_2 = \frac{2^5(-n-4)^{5/2}}{E_F n^4 \sqrt{n^2+16n+128}} .$$

8b. The Error Introduced by this Approximation.

We must now discuss the error involved in keeping only the leading term and also from not including the step function in the exponent when evaluating the saddle point.

Using standard methods, the first few terms in the asymptotic approximation of $\int d\omega_2 \; \phi(\omega_2) \; e^{h(\omega_2)}$ are:

$$(7.63) \quad \phi(\omega_{2_0}) \; e^{h(\omega_{2_0})} a_0 \sqrt{\pi} \; [1 + \frac{(2-1)!!}{2} \frac{a_2}{a_0} + \frac{3!!}{4} \frac{a_4}{a_0} + \ldots]$$

$$+ \; \phi'(\omega_{2_0}) \; e^{h(\omega_{2_0})} \sqrt{\pi} \quad [\; \frac{3a_1 a_0}{2} \quad \frac{(2-1)!!}{2} + \ldots]$$

$$+ \; \frac{\phi''(\omega_{2_0})}{2} \; e^{h(\omega_{20})} \sqrt{\pi} \quad [\frac{a_0^3(2-1)!!}{2} + \ldots \;]$$

where $\phi'(\omega_{2_0}) = \frac{d}{d\omega_2} \; \frac{\text{Imag (Log } (\hbar\omega_2))}{\pi} \Bigg|_{\omega_2=\omega_{2_0}}$

$$\phi''(\omega_{2_0}) = \frac{d^2}{d\omega_2^2} \; \frac{1}{\pi} \; \text{Imag}\Big(\text{Log } (\hbar\omega_2)\Big) \Bigg|_{\omega_2=\omega_{2_0}}$$

Since the Imag (Log (z)) is not analytic, we must say what we mean by the derivative. We can consider this function as a real function of two variables and take the directional derivative tangent to the path of integration. When we look specifically at the directions involved we find that the result is equivalent to taking the imaginary part of the derivative of the analytic function Log (z). In other words, even though it is usually not valid to interchange Im and $\frac{d}{dz}$, in our case we found that the two operations did commute.

It is quite straightforward to evaluate the coefficients a_i and the derivatives. We find that for small n, i.e. n less than one, the ratio of the terms with Φ' and Φ'' to the first term with Φ is 0.12 independently of n. However, for larger values of n, we find that this ratio becomes dependent on n. In fact, it decreases as $\frac{1}{\pi n}$. We defined n to be $\frac{\hbar\omega'}{E_F}$. For a free gas ω', the plasma frequency, is proportional to the square root of the density. Therefore, n increases as the system becomes more dense and the above ratio decreases. For a free electron gas at metallic densities n is about 2 and the ratio is about 0.02. For a free electron gas at atomic densities the ratio becomes 0.002. If we use the value of n for an atom that we calculate at the end, this ratio becomes ~ 0.00002. This ratio represents the error introduced by not including $\Phi(\omega_2)$ in the calculation of the saddle point. We see that for very small densities the maximum error is 12 percent and for very dense systems the error becomes negligible. Since we are interested primarily in very dense systems, this is a very good approximation.

We find that the ratios $\frac{a_2}{a_0}$, $\frac{a_4}{a_0}$ do not depend on n, nor any other parameter in the problem. These numerical coefficients decrease fast enough by themselves to warrant taking only the first term. However we find that

$$\left|\frac{a_2}{a_0}\right| = 0.04 \qquad \text{and} \qquad \frac{(2-1)!!}{2}\left|\frac{a_2}{a_0}\right| = 0.02 .$$

Although this is small enough to justify keeping only the first term, it limits the accuracy we can expect from our final answer.

Repeating the same procedure for the x integration, we again find that the ratios of the terms in the asymptotic series to the first term depend only on the numerical coefficients which fall off quite rapidly.

$$\left|\frac{a_2}{a_0}\right| \sim \frac{1}{20} , \qquad \left|\frac{a_4}{a_0}\right| \sim \frac{1}{1000} ,$$

and

$$\frac{(2-1)!!}{2} \left|\frac{a_2}{a_0}\right| \sim \frac{1}{40} = 0.025 .$$

The total error is less than or equal to the sum of the errors from the ω_2 part and the x part. Therefore, the error introduced by keeping only leading terms should be less than 4.5%.

8c. Comparison of the Path of Steepest Descent with the Correct Path of Integration.

Since we are keeping only the leading term, the direction of the path of steepest descent is just the direction of steepest descent in the region of the saddle. The condition for this path is

(a) $h''(\omega_{2_0})(\omega_2 - \omega_{2_0})^2$ = negative real number

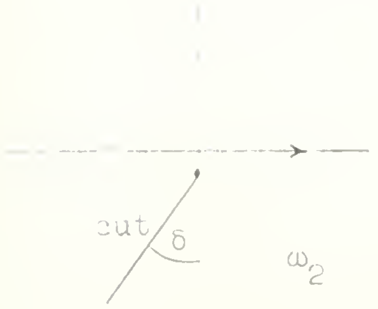
(b) $h''(x_0)\ (x-x_0)^2$ = negative real number.

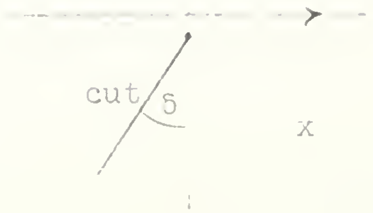
Upon evaluating $h''(\omega_{2_0})$ and $h''(x_0)$ we find that they are both negative real numbers. We write $(\omega_2-\omega_{2_0})^2$ as $\rho^2 e^{2i\theta}$ and $h''(\omega_{2_0})$ as $|R|e^{i\pi}$. From equation (a) we have

$$\pi + 2\theta = \pi \, , \qquad \theta = 0 \, ,$$

so that the path of steepest descent in the ω_2 plane is just a horizontal line through the saddle point. We find the same result for the x plane.

The original paths of integration were also horizontal.



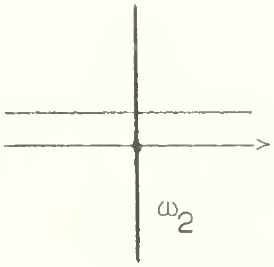


In addition, they lie above the real axis. This is important because there is a singularity at the origin. We have found that the saddle points were

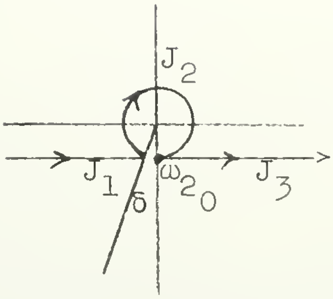
$$\omega_{2_0} \sim \frac{2i}{E_F n} \, , \qquad x_0 = \frac{i\,8(\frac{n}{4}-1)}{E_F n^2} \, .$$

Consider just the ω_2 plane as similar remarks will hold for the x plane. If n is real and positive, then ω_{2_0} lies on the positive imaginary axis. In this case, the path of steepest descent coincides perfectly with the original path and no correction is needed. However, in our problem, we do have terms with n a negative real number.

In such cases ω_{2_0} lies on the negative real axis and the steepest path is then:



We note that this path is on the wrong side of the singularity. Also, it is not permissible to cross the branch cut. Therefore, we must add correction terms to this path.



Choosing the angle δ infinitesimally small, the contributions for J_1 and J_3 are just that from the path of steepest descent. However, the contribution from J_2 must be added on to the value for the integral previously derived.

The evaluation of the contribution from J_2 is just as hard as doing the original integral. However, the problem was avoided in the following way. In the free gas case we know the correct answer and we say:

correct answer = expression (7.62) + correction from J_2.

We evaluate the expression (7.62) in the limit $k \rightarrow 0$, and compare this with the exact answer in the same limit. With

$$n_p^2 = \frac{h^2}{E_F^2}\,\frac{4\pi\rho e^2}{m} = \frac{e^2}{h^2}\,\frac{1}{\rho^{1/3}}\,\frac{\pi^{1/3}\,m}{3^{4/3}}\ , \quad \rho \text{ is the density;}$$

$$E_F = \frac{h^2}{2m}\left(\frac{3\rho}{8\pi}\right)^{2/3} .$$

The expression for (7.62) for $\mu(\omega')$ as $k \rightarrow 0$ has two terms. One becomes proportional to n_p^2/n^2. The exact answer in this limit is n_p^2/n^2. The second term is singular in $1/k^2$. In the exact answer, there is also an apparent singularity in $1/k^2$. But as $k \rightarrow 0$ the numerical coefficients in the exact case are such that the terms with $1/k^2$ all cancel.

Therefore, the expression (7.62) differs from the exact answer as $k \rightarrow 0$ not in any physical constants, but only in numerical coefficients. Therefore, the form of the correction due to J_2 must be the same as the form of $\mu(\omega')$ in (7.62), but with numerical coefficients such that (7.62) + J_2 = exact answer. After doing the arithmetic, this numerical factor is

$$[-1 + c\ i]\ ,$$

where

$$c = \frac{1}{12.3\,F}$$

$$F = \left[\frac{3(-n_p-4)^2}{n_p \sqrt{n_p^2+16n_p+128}} + \frac{(n_p-4)^2}{n_p \sqrt{n_p^2-16n_p+128}} \right]$$

$$n_p = \frac{\hbar^2\, 4\pi\, \rho\, q^2}{E_F^2 \lambda m} \quad , \qquad \rho = \text{density};$$

for metallic densities $c = 0.02183$

for atomic densities $c = 0.02836.$

The contribution due to the J_2 term is just

(7.64) $$[-1 + c\,i] \cdot \mu(\omega')_{\text{from (7.62)}} \cdot$$

9. The Integration Completed for the General Case.

We now refer back to the expressions (7.39), (7.36), and (7.38). It is desired to complete the calculation of $\bar{\mu}(\omega')$ by performing the integrals over ω_1 and ω_2. In (7.36), I_1 and I_2 are independent of ω_1 and ω_2. Define a z_3 and z_4 so that

$$I_3 = (\omega_1 + \omega_2) z_3$$

$$I_4 = (\omega_1^3 + \omega_2^3) z_4$$

where z_3 and z_4 are independent of ω_1 and ω_2. We repeat the same methods now as we used for the free gas case. The calculation falls into two parts. The first is the method of steepest descents. Apart from slightly more difficult algebra, the procedure is exactly the same as before and needs no further discussion. As was mentioned in the free gas case though, we did assume here that

$$\text{(a)} \qquad \frac{u^2 \hbar^2}{E_F N\, 2m} \ll 1 \quad ,$$

(7.52)

$$\text{(b)} \qquad \frac{(u+\beta)^2 \hbar^2}{E_F N\, 2m} \ll 1 \quad .$$

Also, apart from the $\theta(-\hbar\omega_2)$ function, it was possible to include the entire function in the saddle point calculation of each term. (The saddle point differed for the different terms, of course.) To include the error function, use was made of the above approximations (a) and (b) and also of the approximation

$$\Phi(x) \sim \frac{2}{\sqrt{\pi}}\, e^{-x^2} [x + \frac{2x^3}{3} + \ldots]$$

which is valid for small x.

The second part concerns the correction to the path of steepest descent when that path was on the wrong side of the singularity. We know what this correction had to be in the free gas case. Now, when we compare the integrands in $\bar{\mu}(\omega')$ in the general case with equation (7.47) we see that the different terms in $\bar{\mu}(\omega')$ differ from equation (7.47) only in the following ways:

(1) k^2 is replaced by either $-\alpha^2$ or $-(\alpha+\beta)^2$

(2) sometimes there are positive integer powers of x as extra factors

(3) sometimes there is an extra factor of $\sqrt{x}$

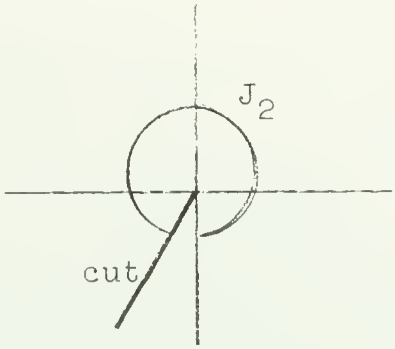
(4) the terms with z_3 have the additional factor $(\omega_1+\omega_2)$.

We should remark here that the terms with z_4 do not have a singularity in ω_2 or x and so we need not consider any correction to these terms.

We can rewrite equation (7.47) as

$$(7.65)\quad \int dx \int d\omega_2 \, \frac{(\omega_2-x)^{1/2}}{\omega_2^3} \, e^{-iE_F\left(\frac{\omega_2^2}{\omega_2-x}+n\omega_2\right)} \, e^{\frac{ik^2\hbar^2 x}{2m}} \cdot \lim_{\varepsilon\to 0} e^{\varepsilon\sqrt{x}} \, (-\hbar\omega_2) \,.$$

The correction was evaluated over a path J_2 in the x and ω_2 planes.



On the path J_2, all the terms of the integrand of (7.65) are bounded as is the path length on J_2. Therefore, equation (7.65) is uniformly convergent. Uniform convergence is sufficient to insure that it is exactly correct to interchange limits, integrations, and differentiations. To find the correction to equation (7.65) due to J_p, we re-evaluate the free gas case with the extra factor $\lim_{\varepsilon \to 0} e^{\varepsilon \sqrt{x}}$ in the integrand.

We find that the correction term for equation (7.65) now becomes

$$(7.66)\quad \lim_{\varepsilon \to 0} \; [-1+ci]\pi \; K \sqrt{\frac{4}{5}} \; \frac{1}{i} \; \frac{[\frac{5i}{2g} + \gamma\varepsilon] e^{-ig[\frac{5i}{2g} + \alpha\varepsilon]} e^{\varepsilon\sqrt{\frac{5i}{2g}}}}{[\frac{5i}{2g} + \alpha\varepsilon]^{5/2}}$$

$$\cdot \; \theta\left(-\frac{\hbar n}{n-4}\left(\frac{5i}{2g} + \alpha\varepsilon\right)\right) ,$$

$$\alpha = \sqrt{\frac{10ig}{4g^2}} , \qquad \gamma = -\frac{(\frac{5i}{2g})^{3/2}}{20} + \alpha$$

$$\left.\begin{matrix} g = g_1 \\ K = K_1 \end{matrix}\right\} \text{if } n > 0 \; ; \qquad \left.\begin{matrix} g = g_2 \\ K = K_2 \end{matrix}\right\} \text{if } n < 0 \; .$$

Referring to equation (7.65) we can evaluate the corrections to each of the terms in the general case by the following procedures.

(1) replace k^2 by $-\alpha^2$ or $-(\alpha+\beta)^2$ as the case may be

(2) if there are extra powers of x, differentiate equation (7.66) by $d/d[k^2\hbar^2/2m]$ for each power in x. This is equivalent to d/dg in equation (7.66).

(3) if there is a factor $\sqrt{x}$ differentiate (7.66) with respect to ε before takimg $\lim_{\varepsilon \to 0}$.

(4) $e^{-iE_F(\frac{\omega_2^2}{\omega_2 - x} + n\omega_2)} = e^{-iE_F(\omega_1 + \omega_2)} \, e^{-i\omega'\omega_2}$.

So for a factor $(\omega_1+\omega_2)$, differentiate equation (7.66) with respect to E_F.

This procedure is quite lengthy, but quite straightforward and not at all difficult. However, it has the obvious disadvantage that taking many derivatives generates many terms. Therefore the final result for $\bar{\mu}(\omega')$ in the general case is very cumbersome.

After carrying out all the procedures indicated in the last few pages we find for $\bar{\mu}(\omega')$:

$$\bar{\mu}(\omega') = [2T(-n) - 2U(+n) - 2U(-n)] , \tag{7.67}$$

where $T(n) = U(n)$ with all the θ functions equal to 1 and all the derivatives of θ equal to 0.

$$\begin{aligned} U(n) = {} & \frac{2^{15}\sqrt{2}\, m^{5/2}\, q^2\pi^3\, i\alpha\beta[I_1+I_2]}{h^5\sqrt{\pi}} \\ & \cdot\left\{\frac{\hbar^2\pi^2 c\, i\sqrt{2}\, K\, e^{5/2}\, g_1^{3/2}\, \theta\left(\frac{\hbar n}{n-4}\frac{5i}{2g_1}\right)}{m\, 2^9\, \beta^4\, 5^2}\right. \\ & - \frac{2\hbar^2\pi^2(\alpha+\beta)c\, i\, K\sqrt{2}\, e^{5/2}\, g^{3/2}\, \theta(g_2)}{\alpha\, 2^{10}\, \beta^4\, m\, 25} \\ & + \frac{2\hbar^2\pi^2\, c\, i\, K\sqrt{2}\, e^{5/2}\, (E_FN)^{3/2}\, \theta(E_FN)}{\alpha\, 2^{10}\, \beta^3\, m\, 5^2} \\ & + \frac{\hbar^2\pi^2 K\, g_1^{3/2}\, 2^{5/2}\, e^{5/2}\, \underline{\Phi}(\alpha\hbar\sqrt{5/16mg_1})\, \theta(g_1)}{2^9\, \beta^4\, 4m\, 25} \\ & - \frac{\hbar^2\pi^2(\alpha+\beta)K\, g_2^{3/2}\, 2^{5/2}\, e^{5/2}\, \underline{\Phi}((\alpha+\beta)\hbar\sqrt{5/16mg_2}\, \theta(g_2))}{2^9\, \alpha\, \beta^4\, 4m\, 25} \end{aligned} \tag{7.68}$$

$$+ \frac{\hbar^3 \pi^{3/2}\ K\ e^{5/2}\ (E_F N)^{3/2}\ \sqrt{-i}\ \theta_g(E_F N)(3\alpha+\beta)}{25\ \alpha\ 2^{10}\ \beta^3\ m^{3/2}}$$

$$+ \frac{\hbar^3 \pi^{3/2}\ K\ e^{5/2}\ E_F N\ z\ \theta(E_F N)\ (3\alpha+\beta)}{25\ \alpha\ 2^{10}\ \beta^3\ m^{3/2}}$$

$$+ \frac{\pi^{3/2}(\alpha+\beta)\hbar^3\ K\ \sqrt{2}\ E_F N\ e^2\ \theta(\frac{\hbar n}{n-4}\ \frac{2i}{E_F N})}{\alpha\ 2^{10}\ \beta^3\ 16\ m^{3/2}}$$

$$- \frac{(\alpha+\beta)^2 \hbar^4 \pi^2\ K\ \sqrt{2}\ g_2^{1/2}\ e^{3/2}\ \theta(\frac{\hbar n}{n-4}\ \frac{3i}{2g_2})}{3\ \alpha\ 2^{10}\ \beta^3\ 8m^2}$$

$$- \frac{(\alpha+\beta)^2 \hbar^4 \pi^2\ \sqrt{2}\ K\ 3\ g_2^{1/2}\ e^{5/2}(-1-ci)\theta(g_2)}{25\ \alpha\ 2^{10}\ \beta^3\ 8m^2}$$

$$- \frac{ic(\alpha+\beta)^2 \hbar^4 \pi^2\ \sqrt{2}\ K\ 3e^{5/2}\ (E_F N)^{1/2}\ \theta(E_F N)}{25\ \alpha\ 2^{10}\ \beta^3\ 8m^2}$$

$$- \frac{(\alpha+\beta)^2 \pi^2 \hbar^4\ K\ \sqrt{2}\ g_2^{3/2}\ e^{5/2}\ \theta_g(g_2)\ (-1-ci)}{25\ \alpha\ 2^{10}\ \beta^3\ 4m^2}$$

$$- \frac{ci(\alpha+\beta)^2 \hbar^4 \pi^2\ K\ \sqrt{2}\ (E_F N)^{3/2}\ e^{5/2}\ \theta_g(E_F N)}{25\ \alpha\ 2^{10}\ \beta^3\ 4m^2}$$

$$+ \frac{(\alpha+\beta)^2 \pi^2 \hbar^4\ \sqrt{2}\ K\ g_2^{1/2}\ \frac{2}{3}\ e^{3/2}\ \Phi(\hbar(\alpha+\beta)\ \sqrt{3/16 g_2 m})\ \theta(\frac{\hbar n}{n-4}\ \frac{3i}{2g_2})}{\alpha\ 2^{10}\ \beta^3\ 16m^2}$$

$$- \frac{(\alpha+\beta)^3\ K\ \pi^{3/2}\ \hbar^5\ e^{5/2}\ z\ \theta(E_F N)}{\alpha\ 2^{10}\ \beta^3\ 4m^{5/2}\ 25}$$

$$- \frac{(\alpha+\beta)^3 \; K \; \pi^{3/2} \; \hbar^5 \; E_F N \; e^{5/2} \; z \; \theta_g(E_F N)}{\alpha \; 2^{10} \; \beta^3 \; 4 \; m^{5/2} \; 25}$$

$$\left. - \frac{(\alpha+\beta)^3 \; K \; \pi^{3/2} \hbar^5 \; \sqrt{-i} \; e^{5/2}[\frac{3}{2}(E_F N)^{1/2} \; \theta_\varepsilon(E_F N) \; +(E_F N)^{3/2} \theta_{\varepsilon g}(E_F N)]}{\alpha \; 2^{10} \; \beta^3 \; 4 \; m^{5/2} \; 25} \right\}$$

$$+ \; \frac{2^{15} m^{5/2} q^2 \alpha\beta\pi^3 i \; \sqrt{2} \; z_3}{h^5 \; \sqrt{\pi}}$$

$$\cdot \left\{ \frac{-i\hbar^2\pi^2 L \;\; \sqrt{2} \; e^{3/2} \; g_1^{1/2} \; \theta(\frac{\hbar n}{n-4} \; \frac{3i}{2g_1})}{2^{10} \; \beta^4 \; m \; 3} \right.$$

$$- \frac{\hbar^2\pi^2 c \; \sqrt{2} \; e^{5/2}}{16 \; \beta^4 \; m \; 25} \; [- \; \frac{K \; g_1^{3/2}}{E_F 25} - \frac{g_1^{3/2} \; n \; Q}{E_F^2} + \frac{K}{26} \; 3 \; g_1^{1/2} \; P] \; \theta(g_1)$$

$$- \frac{\hbar^2\pi^2 c \; \sqrt{2} \; K \; e^{5/2} \; g_1^{3/2} \; \theta_{E_F}(g_1)}{2^9 \; \beta^4 \; m \; 25}$$

$$+ \; \frac{i \; L \; \hbar^2 \; \pi^2 \; \sqrt{2} \; g_1^{1/2} \; e^{3/2}}{2^{10} \; \beta^4 \; m} \cdot \frac{1}{3} \; \underline{\Phi}(\alpha\hbar \sqrt{\frac{3}{16 m g_1}} \;) \; \theta(\frac{\hbar n}{n-4} \; \frac{3i}{2g_1})$$

$$+ \; \frac{i \; \hbar^2\pi^2(\alpha+\beta) \; L \; \sqrt{2} \; e^{3/2} \; g_2^{1/2} \; \theta(\frac{\hbar n}{n-4} \; \frac{3i}{2g_2})}{\alpha \; 2^{10} \; \beta^4 \; m \; 3}$$

$$+ \; \frac{\hbar^2\pi^2(\alpha+\beta)c \; \sqrt{2} \; e^{5/2}}{\alpha \; 2^4 \; \beta^4 \; m \; 25} \; [- \; \frac{K \; g_2^{3/2}}{E_F \; 2^5} - \frac{g_2^{3/2} n \; Q}{E_F^2} + \frac{3K}{2^6} \; g_2^{1/2} \; P]\theta(g_2)$$

$$- \frac{\hbar^2\pi^2 c\sqrt{2} \; e^{5/2}}{\alpha \; 2^4 \; \beta^3 \; m \; 25} \; [\; - \; \frac{K(E_F N)^{3/2}}{E_F \; 2^5} - \frac{(E_F N)^{3/2} n \; Q}{E_F \; 2} + \frac{3K}{2^5} \; (E_F N)^{1/2} P]\theta(E_F N)$$

$$+ \frac{\hbar^2\pi^2(\alpha+\beta)c \; \sqrt{2} \; K \; e^{5/2}[g_2^{3/2} \; \theta_{E_F}(g_2) \; - \; (E_F N)^{3/2} \; \theta_{E_F}(E_F N)]}{2^9 \; \alpha \; \beta^4 \; m \; 5^2}$$

$$- \frac{i\, h^2 \pi^2 (\alpha+\beta) \sqrt{2}\, g_2^{1/2}\, e^{3/2}}{\alpha\, 2^{10}\, \beta^4\, m^2}\; [1-i(\alpha+\beta) h \sqrt{\frac{1}{16 m g_2}}\,]\, \theta(\frac{hn}{n-4}\, \frac{i}{2g_2})$$

$$+ \frac{i h^3 \pi^3 (3\alpha+\beta) e^{5/2}\; 2}{\alpha\, 2^{10}\, \beta^3\, m^{3/2}\; 25}\; [- \frac{2^5 N\, Q\, n}{E_F} + L\, \theta_1]\, \theta(E_F N)$$

$$+ \frac{i h^3 \pi^{3/2}\, K\, e^{5/2}\, (3\alpha+\beta)\, E_F N\; 2\; \theta_{E_F}(E_F N)}{\alpha\, 2^{10}\, \beta^3\, m^{3/2}\; 25}$$

$$+ \frac{i h^3 \pi^{3/2}\, (3\alpha+\beta)\, e^{5/2}\, \sqrt{-i}}{\alpha\, 2^{10}\, \beta^3\, m^{3/2}\; 25}\; [K\, \theta_\varepsilon(E_F N)\, \frac{3}{2}(E_F N)^{1/2} P$$

$$- \frac{(E_F N)^{3/2}}{E_F^2}\, 2^5\, Q\, n\, \theta_\varepsilon(E_F N) - \frac{(E_F N)^{3/2} K\, \theta_\varepsilon(E_F N)}{E_F} + (E_F N)^{3/2} K \theta_{\varepsilon_{E_F}}(E_F N)]$$

$$+ \frac{i\, \pi^{3/2}\, L(\alpha+\beta)\, h^3\, e\; \theta(\frac{hn}{n-4}\, \frac{i}{E_F N})}{\alpha\, 2^{12}\, \beta^3\, m^{3/2}}$$

$$- \frac{i(\alpha+\beta)^2 \pi^2 h^4\, L\, \sqrt{2}\, e^{1/2}\, [1-i(\, (\alpha+\beta)\, \sqrt{1/16 m g_2})\,]\, \theta(\frac{hn}{n-4}\, \frac{i}{2g_2})}{\alpha\, 2^{14}\, \beta^3\, m^2\, g_2^{1/2}}$$

$$- \frac{i(\alpha+\beta)^2 h^4 \pi^2\, \sqrt{2}\; 3\; e^{5/2}\, (-1-ci)}{\alpha\, 2^{13}\, \beta^3\, m^2\; 25} \cdot [- \frac{n\, Q\, 2^5}{E_F^2}\, g_2^{1/2}\, \theta(g_2)$$

$$- \frac{K}{E_F}\, g_2^{1/2}\, \theta(g_2) + \frac{K\, \theta(g_2) P}{2 g_2^{1/2}} + K g_2^{1/2}\, \theta_{E_F}(g_2)]$$

$$+ \frac{c(\alpha+\beta)^2 h^4 \pi^2\, \sqrt{2}\, e^{5/2}\; 3}{\alpha\, 2^{13}\, \beta^3\, m^2\; 25}\; [- \frac{n\, Q\, 2^5}{E_F^2}\, (E_F N)^{1/2}\, \theta(E_F N)$$

$$- \frac{K}{E_F}(E_F N)^{1/2} \theta(E_F N) + \frac{K}{2}\, \frac{P \theta(E_F N)}{(E_F N)^{1/2}} + K (E_F N)^{1/2} \theta_{E_F}(E_F N)]$$

$$- \frac{i(\alpha+\beta)^2 \pi^2 \hbar^4 \sqrt{2}\, e^{5/2} (-1-ci)}{\alpha\, 2^{12} \beta^3 m^2\, 25} \left[- \frac{n 2^5 Q}{E_F^2} g_2^{3/2}\, \theta_g(g_2) - \frac{K}{E_F} g_2^{3/2} \theta_g(g_2)\right.$$

$$\left. + \frac{3}{2} K g_2^{1/2} P\, \theta_g(g_2) + K g_2^{3/2}\, \theta_{g_{E_F}}(g_2)\right]$$

$$+ \frac{c(\alpha+\beta)^2 \hbar^4 \pi^2 \sqrt{2}\, e^{5/2}}{\alpha\, 2^{12} \beta^3 m^2\, 25} \left[- \frac{n\, 2^5\, Q}{E_F^2} (E_F N)^{3/2}\, \theta_g(E_F N)\right.$$

$$- \frac{K}{E_F} (E_F N)^{3/2}\, \theta_g(E_F N) + \frac{3}{2} K (E_F N)^{1/2} P\, \theta_g(E_F N)$$

$$\left. + K (E_F N)^{3/2}\, \theta_{g_{E_F}}(E_F N)\right]$$

$$- \frac{i(\alpha+\beta)^3 \pi^{3/2} \hbar^5\, e^{5/2}}{\alpha\, 2^{12} \beta^3 m^{5/2}\, 25} z\left[- \frac{2^5 Q\, n\, \theta(E_F N)}{E_F^2} + K\, \theta_{E_F}(E_F N)\right.$$

$$\left. - \frac{K}{E_F} \theta(E_F N) - \frac{2^5 Q\, n\, N}{E_F} \theta_g(E_F N) + K o\, \theta_g(E_F N) + K E_F N\, \theta_{g_{E_F}}(E_F N)\right]$$

$$- \frac{i(\alpha+\beta)^3 \pi^{3/2} \hbar^5 \sqrt{-i}\, e^{5/2}}{\alpha\, 2^{12} \beta^3 m^{5/2}\, 25} \left[- \frac{2^5 Q\, n}{E_F^2} - \frac{K}{E_F}\right] \left[\frac{3}{2} (E_F N)^{1/2} \theta_\varepsilon(E_F N)\right.$$

$$\left. + (E_F N)^{3/2}\, \theta_{\varepsilon g}(E_F N)\right]$$

$$- \frac{i(\alpha+\beta)^3 \pi^{3/2} \hbar^5 \sqrt{-i}\, e^{5/2} K}{\alpha\, 2^{12} \beta^3 m^{5/2}\, 25} \left[\frac{3}{4} (E_F N)^{1/2} P_1 \theta_\varepsilon(E_F N)\right.$$

$$+ \frac{3}{2} (E_F N)^{1/2}\, \theta_{\varepsilon_{E_F}}(E_F N) + \frac{3}{2} (E_F N)^{1/2} P\, \theta_{\varepsilon g}(E_F N)$$

$$\left.\left. + (E_F N)^{3/2}\, \theta_{\varepsilon g_{E_F}}(E_F N)\right] \right\}$$

$$+ \frac{2^{15} \sqrt{2}\, m^{5/2} q^2 \pi^3\, i \alpha \beta\, z_4}{h^5 \sqrt{\pi}}$$

$$\cdot\Bigg\{\frac{-i\hbar^2\pi^2\ e^{-1/2}\ M}{2^{11}\beta^4 m\ \sqrt{2}\ g_1^{3/2}}\ \theta\left(\frac{\hbar n}{n-4}\ \frac{1}{2ig_1}\right)$$

$$+\ \frac{i\hbar^2\pi^2\ M\ e^{-1/2}}{2^{11}\beta^4\ \sqrt{2}\ m\ g_1^{3/2}}\ \overline{\Phi}\left(\alpha\ \hbar\sqrt{\frac{-1}{16mg_1}}\right)\ \theta\left(\frac{\hbar n}{n-4}\ \frac{1}{2ig_1}\right)$$

$$+\ \frac{i\hbar^2\pi^2(\alpha+\beta)e^{-1/2}M}{\alpha\ 2^{11}\ \beta^4\ m\ \sqrt{2}\ g_2^{3/2}}\ \theta\left(\frac{\hbar n}{n-4}\ \frac{1}{2ig_2}\right)$$

$$-\ \frac{i\hbar^2\pi^2(\alpha+\beta)M_1 e^{-1/2}}{\alpha\ 2^{11}\ \beta^4\ m\ g_2^{3/2}\ \sqrt{2}}\ \overline{\Phi}\left((\alpha+\beta)\hbar\ \sqrt{\frac{-1}{16mg_2}}\right)\ \theta\left(\frac{\hbar n}{n-4}\ \frac{1}{2ig_2}\right)$$

$$+\ \frac{(\alpha+\beta)\hbar^3\pi^{3/2}\ M\ e^{-1}}{\alpha\ 2^{12}\ \beta^3\ m^{3/2}\ (E_FN)^2}\ \theta\left(\frac{\hbar n}{n-4}\ \frac{1}{iE_FN}\right)$$

$$+\ \frac{i\ M\ \pi^2(\alpha+\beta)^2\ \hbar^4\ 9}{\alpha\ 2^{10}\ \beta^3\ 32\ m^2\ g_2^{5/2}\ \sqrt{2}}\ e^{-3/2}\ \theta\left(\frac{\hbar n}{n-4}\ \frac{3}{2ig_2}\right)$$

$$-\ \frac{iM(\alpha+\beta)^2\pi^2\ \hbar^4\ \sqrt{2}\ e^{-3/2}}{\alpha\ 2^{12}\ \beta^3\ m^2\ g_2^{5/2}}\ \frac{3}{2}\ \Phi\left(\hbar(\alpha+\beta)\ \sqrt{\frac{-3}{16mg_2}}\right)\cdot\theta\left(\frac{\hbar n}{n-4}\ \frac{3}{2ig_2}\right)\Bigg\}$$

$$+\ \frac{q^2\ 2^6\sqrt{2}\ m^{3/2}\alpha\,\beta\,\pi^2\ i}{h^3\ \sqrt{\pi}}\cdot\frac{-\pi^2\hbar^2\ g_3^{1/2}K\ e^{3/2}}{(\beta^2-\alpha^2)^2\alpha\ m\ \sqrt{2}\ 3}\ \theta\left(\frac{\hbar n}{n-4}\ \frac{3i}{2g_3}\right)$$

$$-\ \frac{\hbar^2\pi^2\ K\ \sqrt{2}\ e^{5/2}}{(\beta^2-\alpha^2)^2\ m\ \alpha\ 5^2}\ \Big[-\ \frac{3}{2}\ g_3^{1/2}\ \theta(g_3)-\ \frac{3}{2}\ cig_3^{1/2}\ \theta(g_3)$$

$$+\ \frac{3}{2}\ ci(E_FN)^{1/2}\theta(E_FN)\ -\ g_3^{3/2}\theta_g(g_3)-cig_3^{3/2}\theta_g(g_3)+ci(E_FN)^{3/2}\theta_g(E_FN)\Big]$$

$$+\ \frac{K\ \hbar^2\pi^2\ \sqrt{2}\ g_3^{1/2}\ e^{3/2}}{(\beta^2-\alpha^2)^2\ 4\,m\,\alpha}\ \frac{2}{3}\ \overline{\Phi}\left(\alpha\hbar\sqrt{\frac{3}{4mg_3}}\right)\ \theta\left(\frac{\hbar n}{n-4}\ \frac{3i}{2g_3}\right)$$

$$-\ \frac{4\ \pi^{3/2}\ K\ e^{5/2}\ \hbar^3}{(\beta^2-\alpha^2)^2\ 5^2\ m^{3/2}}\ \Big[z\ \theta(E_FN)\ +\ \sqrt{-i}\ \frac{3}{2}\ (E_FN)^{1/2}\ \theta_\varepsilon(E_FN)$$

$$+\ \sqrt{-i}\ (E_FN)^{3/2}\ \theta_{\varepsilon g}(E_FN)\ +\ z(E_FN)\ \theta_g(E_FN)\Big]$$

$$+ \frac{\hbar \ \pi^{3/2} \ K \ e^{2} \ E_F N}{(\beta^2-\alpha^2)^2 \ \alpha^2 \ \sqrt{2m} \ 4} \ \theta\left(\frac{\hbar n}{n-4} \ \frac{2i}{E_F N}\right)$$

$$- \frac{i\hbar \ \pi^{3/2} \ K \ e^{5/2} \ (E_F N) \ 2}{(\beta^2-\alpha^2)^2 \ \alpha^2 \ \sqrt{m} \ 25} \ \left[\theta(E_F N) iz + \frac{1}{\sqrt{-i}} \ \theta_\varepsilon(E_F N)(E_F N)^{1/2}\right]$$

$$- \frac{i \ c \ \pi^2 \ K \ 2 \ \sqrt{2} \ e^{5/2}}{\alpha^3 (\beta^2-\alpha^2)^2 \ 5^2} \ \left[g_3^{3/2} \ \theta(g_3) - (E_F N)^{3/2} \ \theta(E_F N)\right]$$

$$- \frac{\pi^2 \ K \ g_3^{3/2} \ 2^{3/2} \ e^{5/2}}{\alpha^3 (\beta^2-\alpha^2)^2 \ 25} \ \underline{\overline{\Phi}}\left(\alpha\hbar \sqrt{\frac{5}{4mg_3}}\right) \ \theta\left(\frac{\hbar n}{n-4} \ \frac{5i}{2g_3}\right)$$

$$- \frac{\pi^2 \ \hbar^2 \ K \ e^{3/2} \ g_4^{1/2}}{\beta \ (\beta^2-\alpha^2)^2 \ m \ \sqrt{2} \ 3} \ \theta\left(\frac{\hbar n}{n-4} \ \frac{3i}{2g_4}\right)$$

$$- \frac{\hbar^2 \pi^2 \ K \ \sqrt{2} \ e^{5/2}}{(\beta^2-\alpha^2)^2 \ m \ \beta \ 5^2} \ \Big[- \frac{3}{2} \ g_4^{1/2} \ \theta(g_4) \ (1+ci) + \frac{3}{2} \ ci (E_F N)^{1/2} \theta(E_F N)$$

$$- g_4^{3/2} \ \theta_g(g_4) - ci g_4^{3/2} \ \theta_g(g_4) + ci(E_F N)^{3/2} \ \theta_g(E_F N)\Big]$$

$$+ \frac{K\hbar^2 \pi^2 \ \sqrt{2} \ g_4^{1/2} \ e^{3/2}}{(\beta^2-\alpha^2)^2 \ 2m \ \beta \ 3} \ \underline{\overline{\Phi}}\left(\beta\hbar \sqrt{\frac{3}{4mg_4}}\right) \ \theta\left(\frac{\hbar n}{n-4} \ \frac{3i}{2g_4}\right)$$

$$+ \frac{\hbar \ \pi^{3/2} \ K \ e^{2} (E_F N)}{(\beta^2-\alpha^2)^2 \ \beta^2 \ \sqrt{2m} \ 4} \ \theta\left(\frac{\hbar n}{n-4} \ \frac{2i}{E_F N}\right)$$

$$- \frac{i\hbar \ \pi^{3/2} \ K \ e^{5/2} \ (E_F N) 2}{(\beta^2-\alpha^2)^2 \ \beta^2 \ \sqrt{m} \ 25} \ \left[\theta(E_F N) iz - \sqrt{-i} \ \theta_\varepsilon(E_F N)(E_F N)^{1/2}\right]$$

$$- \frac{i \ c \ \pi^2 \ K \ 2 \ \sqrt{2} \ e^{5/2}}{\beta^3 (\beta^2-\alpha^2)^2 \ 5^2} \ \left[(g_4)^{3/2} \ \theta(g_4) - (E_F N)^{3/2} \ \theta(E_F N)\right]$$

$$- \frac{\pi^2 \ K \ g_2^{3/2} \ 2^{3/2} \ e^{5/2}}{\beta^3 (\beta^2-\alpha^2)^2 \ 25} \ \underline{\overline{\Phi}}\left(\beta\hbar \sqrt{\frac{5}{4 \ mg_4}}\right) \ \theta\left(\frac{\hbar n}{n-4} \ \frac{5i}{2g_4}\right)$$

$$+ \frac{ic\pi^2 K\, 4 \sqrt{2}\, e^{5/2}}{(\beta^2-\alpha^2)^3 \alpha\, 5^2} [g_3^{3/2}\, \theta(g_3) - (E_F N)^{3/2}\, \theta(E_F N)]$$

$$- \frac{ic\pi^2 K\, 4 \sqrt{2}\, e^{5/2}}{(\beta^2-\alpha^2)^3 \beta\, 25} [g_4^{3/2}\, \theta(g_4) - (E_F N)^{3/2}\, \theta(E_F N)]$$

$$+ \frac{\pi^2\, K(g_3)^{3/2}\, 2^{5/2}}{(\beta^2-\alpha^2)^3 \alpha\, 25} \bar{\Phi}(\alpha\hbar \sqrt{\frac{5}{4mg_3}})e^{5/2}\, \theta(\frac{\hbar n}{n-4}\, \frac{5i}{2g_3})$$

$$- \frac{\pi^2 K\, g_4^{3/2}\, 2^{5/2}\, e^{5/2}}{\beta(\beta^2-\alpha^2)^3\, 25} \bar{\Phi}(\beta\hbar \sqrt{\frac{5}{4mg_4}})\, \theta(\frac{\hbar n}{n-4}\, \frac{5i}{2g_4})\Bigg\}$$

where we have used the following abbreviations:

$$N = \frac{5}{4} (\frac{n^2}{n-4}) \qquad g_1 = E_F N + \frac{\alpha^2 \hbar^2}{8m} \qquad g_2 = E_F N + \frac{(\alpha+\beta)^2 \hbar^2}{8m}$$

$$g_3 = E_F N + \frac{\alpha^2 \hbar^2}{2m} \qquad g_4 = E_F N + \frac{\beta^2 \hbar^2}{2m} \qquad K = \frac{2^5 (n-4)^{5/2}}{E_F n^4 \sqrt{n^2-16n+128}}$$

$$L = \frac{8(n-4)^{3/2}}{E_F n^2 \sqrt{n^2-16n+128}} \qquad M = \frac{[(n-4)^3 + 2^6]}{2E_F n \sqrt{n^2-16n+128}\, (n-4)^{1/2}}$$

$$O = \frac{-\frac{5}{4} n^2 (n-8)}{(n-4)^2} \qquad P = O + N \qquad z = \sqrt{\frac{5}{2}}\, \frac{1}{20} + \sqrt{\frac{5}{2}} - \frac{i}{\sqrt{10}}$$

$$Q = \frac{\frac{5}{2} (n-4)^{3/2}}{n^4 \sqrt{n^2-16n+128}} - \frac{4(n-4)^{5/2}}{n^5 \sqrt{n^2-16n+128}} - \frac{(n-4)^{5/2}(n-8)}{n^4 (n^2-16n+128)^{3/2}}$$

$$\theta_\varepsilon(x) = \frac{1}{\pi} \text{Imag}(\frac{1}{\sqrt{10i}\, x^{1/2}}) \qquad \theta_g(x) = \frac{1}{\pi} \text{Imag}\, (-\frac{1}{g})$$

$$\theta_{\varepsilon g}(x) = \frac{1}{\pi} \text{Imag}\, \frac{-1}{2 \sqrt{10i}\, x^{3/2}} \qquad \theta_{\varepsilon_{E_F}}(x) = \frac{1}{\pi} \text{Imag}\, \frac{-P}{2 \sqrt{10i}\, x^{3/2}}$$

$$\theta_{g_{E_F}}(x) = \frac{1}{\pi} \text{Imag}\, \frac{P}{x^2} \qquad \theta_{\varepsilon g_{E_F}}(x) = \frac{1}{\pi} \text{Imag}\, \frac{3P}{4 \sqrt{10i}\, x^{5/2}}$$

$$\theta_{E_F}(x) = \frac{1}{\pi} \text{Imag} \left[\frac{4}{(n-4)E_F} - \frac{P}{x}\right]$$

$$\theta(x) = \frac{1}{\pi} \text{Imag Log } (x)$$

except for

$$\theta(g_\mu)_{\mu=1,2,3,4} = \frac{1}{\pi} \text{Imag Log } \left(\frac{\hbar n}{n-4}\left(\frac{5i}{2g_\mu}\right)\right)$$

and

$$\theta(E_F N) = \frac{1}{\pi} \text{Imag Log } \left(\frac{\hbar n}{n-4} \frac{5i}{2E_F N}\right) .$$

CHAPTER VIII

Description of Numerical Methods

The numerical work was done only for method I. In this case, we have a rather complicated expression for $\mu(\omega')$ which must be stationary with respect to the parameters α, β, and also with respect to those parameters appearing in I_1, I_2, I_3 and I_4.

In order to do the numerical work it was necessary to choose a specific form for the external potential. We decided that an atom would be an interesting example of an inhomogeneous electron gas to study. The external potential for an atom would be the Coulomb potential. However, when the problem was formulated, we did not actually calculate the self-consistent correction to the potential as we should have done because of the difficulty involved. However, we know that if we had made this correction, the external potential would be the Hartree potential, which would be a screened Coulomb potential. Therefore, it was decided to choose

$$V(r) = b\ e^{-ar} .$$

For typical atomic parameters we chose those for Krypton. For Krypton the Fermi level (the energy of the highest bound state) is $- 22.4 \times 10^{-12}$ ergs. We let $b = Zq^2/10^{-8}$. For Krypton $Z = 36$ so b is $115.27\ E_F$. We first chose a to be 10^8 and then for a confidence factor we let a be 10^9.

For a potential of the form be^{-ar}, we have already computed I_1, I_2, I_3 and I_4 (see (7.32), (7.33), (7.34) and (7.35)). These terms involve the parameters A and γ. These expressions I_1, I_2, I_3 and I_4 must be substituted into $\mu(\omega')$.

$\mu(\omega')$ must now be stationary with respect to α, β, A and γ. Therefore, we took the partial derivatives of $\mu(\omega')$ with respect to each of these parameters and required these four derivatives to be zero. Since the derivatives with respect to α and β were rather lengthy and so error prone, they were checked numerically. The derivatives of $\mu(\omega')$ with respect to α and β at a point (α_0, β_0) were evaluated numerically by a difference method. These numbers were then checked with the analytical expressions for these derivatives evaluated at the same point (α_0, β_0). In this way we could be sure that the analytical expressions for these derivatives were correct and also that they were programmed correctly. This same method also checked that $\mu(\omega')$ was correctly programmed.

The condition for a resonance was Real $(\mu(\omega')) = 1$. The imaginary part of $\mu(\omega')$ was a measure of the damping. Since we were interested in only observable resonances we required zero damping -- i.e. that Imag $(\mu(\omega')) = 0$ for a real ω'.

We therefore had to solve simultaneously the following six equations:

$$
\begin{aligned}
RF1 &= \text{Real } \mu(\omega') = 1 \\
IF1 &= \text{Imag } \mu(\omega') = 0 \\
F2 &= \frac{\partial \mu(\omega')}{\partial \alpha} = 0 \\
F3 &= \frac{\partial \mu}{\partial \beta} = 0 \\
F4 &= \frac{\partial \mu}{\partial A} = 0 \\
F5 &= \frac{\partial \mu}{\partial \gamma} = 0 \, .
\end{aligned}
\tag{8.1}
$$

for the unknowns n, α, β, A, γ where $n = \frac{\hbar\omega'}{E_F}$.

We then defined a function F to be

$$
F = (RF1 - 1)(RF1 - 1)^* + (IF_1)(IF_1)^* + c_2F_2F_2^* + c_3F_3F_3^* + c_4F_4F_4^* + c_5F_5F_5^* ,
$$

where the c's are positive numbers and the asterisk signifies complex conjugation.

We see that a zero in F corresponds to a solution of all the equations. Furthermore we see from the definition that $F \geq 0$. Therefore to solve the system we minimized F hoping to find that at the minimum F would be zero. Since, in method II we found that the approximations made had an error of 4.5 percent, we decided to count as a zero any values of F that were zero to 3 or more significant figures. The c's were introduced as scaling factors so that each of the separate equations would have equal weight.

If we look at the specific expressions for $F4(\frac{\partial\mu}{\partial A})$ and $F5(\frac{\partial\mu}{\partial\gamma})$ we see that F4 has a γ^3 in the denominator and F5 has a γ^4. We found numerically that these denominators dominated these equations and we were getting solutions for $\gamma \to \infty$. We have shown before (see page 85) that in this case $\mu(\omega')$ reduces to the free gas value. To avoid this solution we therefore replaced F4 and F5 by the numerators of F4 and F5, i.e. we required

$$\text{numerator } F4 = 0 , \qquad \text{numerator } F5 = 0$$

This resulted in a modification of F.

$$F = (RF1 - 1)(RF1 - 1)^* + IF_1IF_1^* + c_2F_2F_2^*$$
$$+ c_3F_3F_3^* + \gamma^3c_4F_4F_4^* + \gamma^4c_5F_5F_5^* .$$

To minimize F we used a routine called BOTM from the CIMS Library. This routine had the advantage of not requiring derivatives and also it converged well even for very poor initial guesses.

It must be mentioned that the following restrictions on the parameters were made:

(1) α,β occur in the expressions for eigenfunctions $e^{-\alpha r}$ and $e^{-\beta r}$. Since it is unphysical for these functions to become infinite as r goes to infinity, we required that the real parts of α and β not be negative.

(2) If the real part of A became more negative than -100 then the value of F became too large for the machine to handle. Since we were looking for a minimum, we knew that the solution for A could not lie in that region. Therefore the real part of A was not allowed to be less than -100.

(3) We were looking for a positive frequency. Since E_F was negative and $n = \frac{\hbar\omega}{E_F}$, we required n to be negative.

CHAPTER IX

Results

Two distinct solutions of equations (8.1) were found. For the first solution we determined the values:

$$n = -16.3$$

$$\alpha = (1.38 \times 10^{7}, -4.87 \times 10^{8})$$ [13]

$$\beta = (1.18 \times 10^{7}, 9.26 \times 10^{8})$$

$$\gamma = (6.47 \times 10^{7}, -1.72 \times 10^{7})$$

$$A = (127.5, -33.4)$$

$$\hbar\omega' = E_F n = 22.4 \times 10^{-22} \times 16.3 =$$

$$= 3.67 \times 10^{-10} \text{ ergs}$$

$$\frac{2\pi c}{\omega'} = 54 \text{ Å}$$

This solution was very unstable with respect to changes in α or β of 0.1 percent.

This highly singular solution reminds us of the breathing mode found in a system of harmonic oscillators which are coupled to a common center and to each other. The second solution was not so sharp. We found the following ranges in the parameters corresponded to a solution:

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[13] The two numbers in parentheses refer to the real and imaginary parts of the parameters.

$n = -1.78 \times 10^3$ to -3.70×10^3

α $(5.28 \times 10^7$ to 1.26×10^8, -4.68×10^8 to $-4.50 \times 10^8)$

β $(3.27 \times 10^8$ to 3.30×10^8, 7.64×10^8 to $8.39 \times 10^9)$

A $(8.32 \times 10^1$ to 4.03×10^1, -1.21×10^2 to $-1.27 \times 10^2)$

γ $(1.18 \times 10^8$ to 1.13×10^8, 1.50×10^7 to $1.98 \times 10^7)$

There is a reason for the lack of sharpness. We found that for the above ranges in the parameters α, β, equations $F_2 = F_3$ i.e. $\frac{\partial\mu}{\partial\alpha} = \frac{\partial\mu}{\partial\beta}$. Therefore, instead of uniqueness in this region there is a family of solutions since the problem is underdetermined.

$\hbar\omega' = E_F n$ ranges from 3.99×10^{-8} to 8.29×10^{-8} ergs

and

$\frac{2\pi c}{\omega'}$ ranges from 0.24 Å to 0.46 Å.

These numbers would indicate a K shell vibration rather than the whole atom and the lack of sharpness would indicate that the vibration of this shell is perturbed by the other shells. Our original ansatz that the solution to our integral equation be an s state may be forcing an s state solution which is not really correct. This shows up as a solution which is not sharp.

CHAPTER X

1. General Remarks

We have shown that two separate collective states may exist in an atom, one at 54 Å and the other between .24 Å and .46 Å. There may be other solutions in addition. Our solutions were found from the zeros of $1-\mu(\omega')$ where $\mu(\omega')$ is an eigenvalue of equation (2.33) corresponding to the s state eigenfunctions $\phi(x') = e^{-\beta|x'|}$ and $\psi(x) = e^{-\alpha|x|}$. There are other eigenvalues corresponding to higher order eigenfunctions. It may be that some of these other eigenvalues will lead to additional collective states. Furthermore, our final solutions were obtained by numerical methods which unfortunately cannot guarantee uniqueness. Therefore, a more extensive numerical search might discover additional collective states even for the $\mu(\omega')$ that we have worked with.

An additional point needs to be discussed concerning the validity of our results with respect to a real atom. In our derivation, we considered a nonuniform dense electron gas perturbed by the interelectron Coulomb force. The nonuniformity was due to a self-consistent external potential which we have shown to be equivalent to a Hartree potential. However, in our application to an atom, we did not use the exact Hartree potential for an atom. Instead, we approximated the density variation typical of an atom by choosing the form of the external potential to be be^{-ar}, with the amplitude b and the range a chosen to approximate an atom. We have answered the question as to whether very nonuniform systems can still have plasma oscillations. In fact, we have shown that an atomic system should show these effects. However, because an exact atomic Hartree potential was not used, our results are probably valid only as an order of magnitude estimate.

2. Comparison with Other Theoretical Work in the Subject.

Unfortunately, there is not much other work to compare with. In fact to our knowledge, there does not exist any work besides ours which includes the damping effects. However, we will discuss those few papers that there are which deal with the subject of collective states in atoms.

Several papers in this subject have been published by W. Brandt and S. Lundqvist. In the first of these papers,[14] the authors consider a response function $R(\vec{q},\omega)$ defined as

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[14] W. Brandt and S. Lundqvist, Phys. Rev. 132, 2135 (1963).

$$(10.1) \qquad R(\vec{q},\omega) = \int d^3x \, d^3x' \, e^{-i\vec{q}\cdot(x-x')} \, Q(x,x',\omega) \; ,$$

with Q given by the integral equation

$$(10.2) \qquad Q = Q_0 + Q_0 v \, Q$$

Q_0 is defined as auto-correlation function in the Hartree-Fock picture and the expression given for Q_0 is exactly the same as our expression for $\overline{V}$ in lowest order. (See equation (5.4).) The resonances of the system correspond to the poles of $R(\vec{q},\omega)$. We note at once the correspondence between (10.1) and (10.2) and our equations (2.27) to (2.32).

The authors try to take into account the effects of a density gradient when evaluating Q_0 by using a formula due to R. Glauber. In so doing, they find that Q_0 depends upon

$$(10.3) \qquad \langle \theta_{\pm} [\bar{p}^2 - p_F^2(\bar{x}) \rangle$$

and that

$$(10.4) \qquad \langle \theta_{\pm}(z) \rangle = \pm \frac{1}{2\pi i} \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} \frac{e^{i(zt-t^3)}}{t \mp i\varepsilon} \, dt \; .$$

This is equivalent to the approximation we have for the density operator. If they had proceeded along these lines, they would have done what we have done. However, in solving the integral equation (10.2), Brandt and Lundqvist use

$$(10.5) \qquad \alpha(q,\omega) = \frac{\alpha_0(q,\omega)}{1 - \frac{4\pi}{q^2}\alpha_0(q,\omega)}$$

which is the same as if we were to use plane waves for our functions Φ and Ψ. They then find that in the long wavelength limit expression (10.4) gives the same result as a gas with no density gradient. This is not surprising to us as we found that our result reduces to the uniform case when we let Φ and Ψ approach plane waves and take the long wavelength limit.

In another paper,[15] Brandt and Lundqvist make use of the result that in the high quantum number limit the properties of an atom can be studied by considering an assembly of coupled harmonic oscillators in which the coupling constants depend upon the mean radii of electron orbitals. Using this model they derive a linear relationship between the total dipole moment of the atom and an externally applied field. From this they determine the atomic polarizability, $\alpha(\omega)$ in terms of the single particle oscillator strengths f_n, excitation frequencies ω_n and coupling constants λ_n. The resonances of the system occur at the poles of $\alpha(\omega)$. With all the λ_n taken at some mean λ they find the disperson relation

$$(10.6) \qquad 1 + \lambda^2\alpha(\omega) = 0 .$$

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[15] W. Brandt and S. Lundqvist, J. Quant. Spect. Rad. Transfer, Vol. 4, pp. 679-689 (1964).

This is equivalent to our condition that the real part of the dielectric constant be zero. The solutions of (10.6) can correspond to single particle as well as collective effects. We found that we needed a second condition i.e. that the imaginary part of the dielectric constant be zero, in order to determine the collective states. By looking at contributions to $\alpha(\omega)$ from the different atomic shells and by qualitative arguments, Brandt and Lundqvist deduce that collective effects should be in the frequency range $1 < (\frac{\omega}{R_y}) < Z^2$ where $\hbar R_y = 13.6$ eV. This would put ω in the range of 10 - 100 Å. Our first solution of 54 Å agrees very well with this result. Our second solution does not. However, at wavelengths shorter than K-shell absorption, the dipole approximation of Brandt and Lundqvist does not suffice. Therefore, it is understandable that their method does not yield a solution at very short wavelengths. We should remark that one of the conditions Brandt and Lundqvist use to determine which of their resonances is collective is that there be "a sufficiently high gap on the high-frequency side of the single particle spectrum of accommodate this new resonance". Our solution of .24 Å to .46 Å satisfies this condition as it lies beneath the K shell.

The problem of collective oscillations in atoms has also been considered by Wieder and Borowitz.[16] They consider the response of the atom to a long wavelength radiation field and use first order time dependent perturbation theory to construct a time dependent Hartree-Fock field from a stationary one. The relationship between the induced electron density fluctuation and the perturbing radiation field is linearized and a multipole expansion performed. The resonances in the induced dipole moment are related to the excited states of the system. The low frequency resonances are identified as single particle excitations while a high frequency collective state is identified in a region where oscillator strengths for single particle transitions are negligible. They find that the collective wavelengths for Krypton, Argon and Neon are [illegible]07 Å, 145 Å and 160 Å respectively.[17] They also find that if a Thomas-Fermi model is used instead of Hartree-Fock, then the collective excitation for Argon is about 5 Å. In this study, the effect of damping was not included so we do not know if the excitations at these frequencies are well defined. Upon comparing these values with ours we see that the agreement is poor. Several reasons could account for this. First, as we have mentioned our results are not unique. It could be that had we considered p state eigenfunctions instead of s state ones we would have found collective modes in agreement with Wieder and Borowitz. The collective states of Wieder and Borowitz are also not unique since they studied in detail only the dipole terms. Higher multipole terms might have given other additional collective states. Secondly, we did not use the exact Hartree potential. Judging from the large discrepancy that Wieder and Borowitz found between the Hartree-Fock solution and a Thomas-Fermi model our approximate potential could be a large source of error. Finally, it could be that the collective state found by Wieder and Borowitz rapidly decays into single particle states. Our results were found by insisting that the damping be small. If we had not demanded this, we could have found solutions in the same range as Wieder and Borowitz.

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[16] S. Wieder and S. Borowitz, Phys. Rev. Letters 16 (1966) 724.

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[17] These numbers do not appear in the published work but are taken from S. Wieder, Ph.D. Thesis, New York Univ., Oct. 1966. The published paper reports a value for Argon only. This value is 20 Å which is quite different from the 195 Å reported in the thesis. The discrepancy is attributed to the paper's being published before the completion of the thesis and contains only rough estimates.

There have also been some Russian papers on the subject. Unfortunately, these papers are all very sketchy and so a detailed discussion is not possible. In one of these papers,[18] it seems that the basic approach resembles ours (see Chapter V). They use trial functions containing 36 parameters and a variational calculation to obtain a collective state for Neon at 68.2 eV. We note that this is in very good agreement with the first of our values.

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[18] Y. Y. Dmitriev, L. N. Labzowsky, Physics Letters 29A (1969) 44.

It is not clear from this paper whether any damping effects were included. There is another paper[19] which alludes to an experiment on inelastic collisions of Argon ions in which three maxima in the cross-section as a function of energy loss were found. The author interprets these maxima as evidence for collective states. Two of the experimental maxima were 40-70 eV and 220-320 eV. The value of the third maximum is not mentioned. The second of these is in close agreement with our first solution of 58 Å.

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[19] M. Ya. Amusia, Physics Letters 14 (1965) 36.

APPENDIX A

An Approximation for the Density Matrix[20]

Suppose $\Gamma(x,p)$ represents a phase space distribution function. Then the expectation value of $f(\bar{x},\bar{p})$ is

$$\text{(A.1)} \qquad \langle f(\bar{x},\bar{p})\rangle = \int\int f(x,p)\,\Gamma(x,p)\,dx\,dp \ ,$$

where the bars signify operators. We can write

$$\text{(A.2)} \qquad f(\bar{x},\bar{p}) = \int e^{\frac{1}{2}\frac{i\bar{p}q}{\hbar}} f_q(\bar{x})\, e^{\frac{1}{2}\frac{i\bar{p}q}{\hbar}}\, dq \ .$$

We note that

$$e^{\frac{1}{2}\frac{i\bar{p}q}{\hbar}} f_q(\bar{x}) = e^{\frac{q}{2}\frac{\partial}{\partial x}} f_q(x)$$

$$= f_q(x + \tfrac{q}{2})\, e^{i\bar{p}q/2\hbar} ,$$

so that

$$\text{(A.3)} \qquad f(\bar{x},\bar{p}) = \int f_q(\bar{x} + \tfrac{q}{2})\, e^{\frac{i\bar{p}q}{\hbar}}\, dq \ .$$

If we take the expectation value of $f(\bar{x},\bar{p})$ we have

$$\text{(A.4)} \quad \langle f(\bar{x},\bar{p})\rangle = \iiint \psi^*(x)\, f_q(x + \tfrac{q}{2}) e^{\frac{i\bar{p}q}{\hbar}}\, e^{\frac{ixp}{\hbar}}\, \psi_p\, dx\,dp\,dq \ ,$$

which is the same as

$$\text{(A.5)} \quad \langle f(\bar{x},\bar{p})\rangle = \iiint \psi^*(x - \tfrac{q}{2})\, f_q(x)\, e^{\frac{i\bar{p}q}{\hbar}}\, e^{i(x - \frac{q}{2})\frac{p}{\hbar}}\, \psi_p\, dx\,dp\,dq$$

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[20] This approximation is based upon work done by John Snygg, Ph.D. Thesis, Courant Inst. Math. Sci., New York Univ., 1967.

Integrating over p gives

$$\langle f(\bar{x},\bar{p})\rangle = \int \psi^*(x-\tfrac{q}{2})\, f_q(x)\, \psi(x+\tfrac{q}{2})\, dx\, dp \tag{A.6}$$

$$= \int \psi^*(x-\tfrac{q}{2})\, f(x,p)\, e^{-\frac{ipq}{\hbar}}\, \psi(x+\tfrac{q}{2})\, dx\, dp$$

We see then, upon comparing, (A.1) with (A.6), that the phase space distribution function is

$$\Gamma(x,p) = \int e^{-\frac{ipq}{\hbar}}\, \psi^*(x-\tfrac{q}{2})\, \psi(x+\tfrac{q}{2})\, dq\ . \tag{A.7}$$

This expression is generally known as the Wigner density. If $x_1 = x + q/2$, $x_2 = x - q/2$,

$$\Gamma(\frac{x_1+x_2}{2},p) = \int e^{-\frac{ip(x_1-x_2)}{\hbar}}\, \psi^*(x_2)\psi(x_1)\, dq \tag{A.8}$$

or

$$\Gamma(\frac{x_1+x_2}{2},p) = \int e^{-\frac{ip(x_1-x_2)}{\hbar}}\, \rho(\vec{x}_1,\vec{x}_2)\, dq\ , \tag{A.9}$$

where $\rho(\vec{x}_1,\vec{x}_2)$ is the Dirac density.

Hence, we can express the Dirac density in terms of the Wigner density.

$$\rho(\vec{x}_1,\vec{x}_2) = \int e^{ip(x_1-x_2)/\hbar}\, \Gamma(\frac{x_1+x_2}{2},p)\, dp\ . \tag{A.10}$$

This expression is useful because it is easier to develop a closed form for the Wigner density than for the Dirac density. In order to arrive at a closed form expression for the Wigner density the following identity proved useful:

(A.11) $$\Gamma(x,p) = \frac{1}{8}\,\mathrm{Tr}\,(\rho(\bar{x} + X,\ \bar{p} + P)\,R\,)$$

where the unbarred letters are c numbers, the barred letters are operators, and R is the reflection operator.

We would now like to show that this expression is the same as (A.7). We can rewrite (A.11) as

(A.12) $$\Gamma(x,p) = \mathrm{Tr}\ e^{-i\bar{x}\cdot P/\hbar}\ e^{i\bar{p}\cdot X/\hbar}\ \rho(\bar{x},\bar{p})\ e^{-\frac{i}{\hbar}\bar{p}\cdot X}\ e^{\frac{i}{\hbar}\bar{x}\cdot P}\ R\ .$$

Evaluating the trace gives

(A.13) $$\Gamma(x,p) = \int \langle x'|e^{-i\bar{x}\cdot P/\hbar\ +i\bar{p}\cdot X/\hbar}|x''\rangle\langle x''|\rho(\bar{x},\bar{p})|x'''\rangle$$

$$\cdot\langle x'''|e^{-i\bar{p}\cdot X/\hbar\ +i\bar{x}\cdot P/\hbar}|x^{iv}\rangle\langle x^{iv}|R|x'\rangle\ dx'dx''dx'''dx^{iv}$$

Now

$$\langle x'|e^{-i\bar{x}\cdot P/\hbar\ +i\bar{p}\cdot X/\hbar}|x''\rangle = e^{-ix'\cdot p/\hbar}\ \delta(x'-x''+X)$$

and

$$\langle x'''|e^{-i\bar{p}\cdot X/\hbar\ +i\bar{x}\cdot P/\hbar}|x^{iv}\rangle = e^{ix^{iv}\cdot P/\hbar}\ \delta(x'''-x^{iv}-X)$$

and

$$\langle x^{iv}|R|x'\rangle = \delta(x' + x^{iv})$$

so (A.13) becomes

(A.14) $$\Gamma(x,p) = \int \langle X+x'|\rho|X-x'\rangle\ e^{-\frac{i}{\hbar}2x'\cdot P}\ dx'\ .$$

Let $x' = \frac{1}{2}\,y$.

(A.15) $$\Gamma(x,p) = \frac{1}{8}\int \langle X-\tfrac{1}{2}\,y|\rho|X+\tfrac{1}{2}\,y\rangle\ e^{-\frac{i}{\hbar}y\cdot P}\ dy$$

which is the same as (A.7).

The bare density operator is $\theta(E_F - H)$ where θ is the step function, E_F is the Fermi energy, and $H = \frac{p^2}{2m} + U$. Using an integral representation for the step function we have

$$(A.16)\qquad \rho(\bar{x},\bar{p}) = -\frac{1}{2\pi i}\int \frac{e^{-i\omega(E_F - \frac{\bar{p}^2}{2m} - U(\bar{x}))}}{\omega + i\varepsilon}\, d\omega$$

and

$$(A.17)\qquad \rho(\bar{x}+X,\bar{p}+P) = -\frac{1}{2\pi i}\int \frac{d\omega}{\omega+i\varepsilon}\, e^{-i\omega(E_F - \frac{(\bar{p}+P)^2}{2m} - U(\bar{x}+X))}$$

If U is slowly varying,

$$U(\bar{x}+X) \cong U(X) + \vec{\nabla} U(X)\cdot\bar{x}$$

If we substitute this into (A.11), we have

$$(A.18)\qquad \Gamma(X,P) = -\frac{1}{2\pi i}\int \frac{d\omega}{\omega+i\varepsilon}\, e^{-i\omega(E_F - \frac{P^2}{2m} - U(X))}$$

$$\cdot\ \frac{1}{6}\,\mathrm{Tr}\; e^{i\omega(\frac{\bar{p}^2}{2m} + \frac{P\cdot\bar{p}}{m} + \nabla U(X)\cdot\bar{x})}\ R\ .$$

let $\vec{\gamma} = \nabla\vec{U}(x)$; let

$$A = \vec{\gamma}\cdot\bar{x} = \sum_j i\omega\gamma_j r_j\ , \qquad B = \frac{i\omega p^2}{2m} + i\omega\sum_k \frac{P_k\bar{p}_k}{m}$$

$$(A.19)\qquad e^{(A+B)} = e^{A}\, e^{(B + \frac{1}{2}[B,A] + \frac{1}{6}[[B,A],A])}$$

since the higher order commutators vanish.

$$[B,A] = -\omega^2\sum_j \gamma_j[\frac{\bar{p}^2}{2m}, \bar{r}_j] - \frac{\omega^2}{m}\sum_j \gamma_j P_k[\bar{p}_k, \bar{r}_j]$$

$$(A.20)\qquad [B,A] = \sum_j \frac{\hbar i\omega^2}{m}\gamma_j\bar{p}_j + i\hbar\omega^2\sum_j \gamma_j P_j$$

$$\text{(A.21)} \quad [[B,A],A] = -\frac{\hbar\omega^3}{m}\sum_j\sum_k \gamma_j\gamma_k\,[\bar{p}_j, r_k] = \frac{i\hbar^2\omega^3}{m}\sum_j \gamma_j^2 \,.$$

Using equations (A.19), (A.20) and (A.21) to evaluate the trace in (A.18) we have

$$\text{(A.22)} \quad \int \langle p'|\, e^{[i\omega\Sigma_i\gamma_i\bar{r}_i]} \exp\Big[\frac{i\omega\bar{p}^2}{2m} + i\omega\sum_i \frac{P_i\bar{p}_i}{m} +$$

$$+ \frac{1}{2}\,\frac{i\hbar\omega^2}{m}\sum_i \gamma_i\bar{p}_i + \frac{i\hbar\omega^2}{2m}\sum_i \gamma_i P_i + \frac{i\hbar^2\omega^3}{6m}\sum_i \gamma_i^2\Big]\,|-p'\rangle\, d^3p' .$$

Since $e^{i\omega\Sigma_i\gamma_i\bar{r}_i}$ is just a Taylor operator on the state $|p'\rangle$, and $\bar{p}|-p'\rangle = -p'|-p'\rangle$, (A.22) is equal to

$$\text{(A.23)} \quad \int d^3p\, \langle p'-\omega\gamma\hbar|\exp\Big[\frac{i\omega p'^2}{2m} - \frac{i\omega P\cdot p'}{m} - \frac{i\hbar\omega^2\gamma\cdot P'}{2m}$$

$$+ \frac{\omega^2\gamma\cdot P i\hbar}{2m} + \frac{i\hbar^2\omega^3\gamma^2}{6m}\Big|\; -p'\rangle \,.$$

Since we have only c numbers now, the only nonzero contribution is when

$$\text{(A.24)} \qquad p' - \omega\gamma\hbar = -p' \quad \text{or} \quad p' = \frac{\omega\gamma\hbar}{2} \,.$$

Using (A.24), the exponent in (A.23) becomes

$$\text{(A.25)} \qquad \exp\Big[\frac{i\hbar^2\omega^3\gamma^2}{24\,m}\Big]$$

which is $\exp\Big[\frac{i\hbar^2\omega^3|\nabla U(x)|^2}{24\,m}\Big]$ since $\vec{\gamma} = \overrightarrow{\nabla U(x)}$

If we use correct δ function normalization, (A.23) also contributes the multiplicative factor, $2^3/h^3$.

Substituting back into (A.18) gives

$$(\text{A.26}) \quad \Gamma(x,p) = \frac{-2}{h^3}\frac{1}{2\pi i}\int \frac{d\omega}{\omega + i\varepsilon}\left[e^{-i\omega(E_F - \frac{p^2}{2m} - U(x))} \cdot e^{i\hbar^2\omega^3 |\nabla U(x)|^2/24m}\right]$$

where we have multiplied by 2 to account for spin.

Therefore, for a slowly varying potential, the Dirac density is

$$(\text{A.27}) \quad \rho(x_1,x_2) = \frac{-2}{h^3}\;\frac{1}{2\pi i}\int \frac{d\omega}{\omega + i\varepsilon}\; e^{i\vec{p}\cdot(\vec{x}_1 - \vec{x}_2)} \cdot e^{i\omega(E_F - \frac{p^2}{2m} - U(\bar{x}) + \frac{i\omega^3\hbar^2}{24m}|\nabla U(\bar{x})|^2}\;,$$

where $\bar{x} = \dfrac{x_1 + x_2}{2}$.

APPENDIX B

The Evaluation of Some Integrals which Appear in Method II

Consider the integrals over $\vec{k}_1$ and $\vec{k}_2$, for the terms I_1, I_2, I_3 and $I4$.

$$(B.1) \quad \int_{-\infty}^{\infty} d^3k_1 \int_{-\infty}^{\infty} d^3k_2 \, \frac{\alpha}{(k_1^2+\alpha^2)^2} \, \frac{\beta}{(k_2^2+\beta^2)^2 k_2^2} \, e^{\frac{i|\overrightarrow{k_1-k_2}|^2 \hbar^2 \omega_1 \omega_2}{8m(\omega_1+\omega_2)}}$$

$$= \int_0^{\infty} 4\pi k_1^2 \, dk_1 \int_0^{\infty} 2\pi k_2^2 \, dk_2 \int_{-1}^{1} d \cos \theta_{12}$$

$$\cdot \; \frac{\alpha}{(k_1^2+\alpha^2)^2} \, \frac{\beta}{(k_2^2+\beta^2)^2 k_2^2} \, e^{i[k_1^2+k_2^2-2k_1 \cdot k_2] \frac{\hbar^2}{8m} \frac{\omega_1 \omega_2}{\omega_1+\omega_2}}$$

$$= \frac{8m(\omega_1+\omega_2) 8\pi^2 \alpha \, \beta}{\hbar^2 \omega_1 \omega_2 \, 2i} \int_0^{\infty} dk_1 \int_0^{\infty} dk_2 \, \frac{k_1 k_2}{(k_1^2+\alpha^2)^2 (k_2^2+\beta^2)^2 k_2^2}$$

$$\cdot \; [e^{\frac{i\omega_1 \omega_2 \, \hbar^2}{(\omega_1+\omega_2) 8m} (k_1+k_2)^2} - e^{\frac{i\omega_1 \omega_2 \, \hbar^2}{8m(\omega_1+\omega_2)} (k_1-k_2)^2}]$$

Let $u = k_1+k_2$, $v = k_1-k_2$, $k_1 = \frac{u+v}{2}$, $k_2 = \frac{u-v}{2}$.

The Jacobian = 1/2.

Also note that

$$(B.2)\quad \int_0^\infty dk_1 \int_0^\infty dk_2 \, \frac{k_1k_2}{(k_1^2+\alpha^2)^2(k_2^2+\beta^2)^2k_2^2} \cdot \left[e^{\frac{i\omega_1\omega_2\hbar^2}{(\omega_1+\omega_2)8m}(k_1+k_2)^2} - e^{\frac{i\omega_1\omega_2\hbar^2}{(\omega_1+\omega_2)8m}(k_1-k_2)^2} \right]$$

$$= \frac{1}{2}\int_{-\infty}^\infty dk_1 \int_{-\infty}^\infty dk_2 \, \frac{k_1k_2}{(k_1^2+\alpha^2)^2(k_2^2+\beta^2)^2k_2^2} \, e^{\frac{i\omega_1\omega_2\hbar^2}{(\omega_1+\omega_2)8m}(k_1+k_2)^2}$$

$$(k_1^2+\alpha^2) = (k_1+i\alpha)(k_1-i\alpha).$$

We get

$$(B.3)\quad \frac{8\pi^2m(\omega_1+\omega_2)}{\hbar^2\omega_1\omega_2 \, i} \int_{-\infty}^\infty \int_{-\infty}^\infty \left\{ du\, dv \cdot \frac{4^4 \, e^{\frac{i\hbar^2\omega_1\omega_2u^2}{8m(\omega_1+\omega_2)}} (u+v)\alpha\,\beta}{(u-v)[u+v+2i\alpha]^2[u+v-2i\alpha]^2[u-v+2i\beta]^2[u-v-2i\beta]^2} \right\}$$

The integration over v was performed by contour integration. Note that there is a singularity at v = u which corresponds to $k_2 = 0$. The original integral did not have a singularity at $k_2 = 0$; the singularity was introduced artificially by the transformations made. I therefore excluded v = u from within the contour. The result after integrating over v is

$$(B.4)\ \int_{-\infty}^{\infty} du\ \frac{2\pi^3 4^4\ 8m(\omega_1+\omega_2)}{\hbar^2\omega_1\omega_2}\ e^{\frac{i\omega_1\omega_2\hbar^2u^2}{8m(\omega_1+\omega_2)}}\ \alpha\ \beta$$

$$\cdot\left\{ \frac{1}{(2u-2i\alpha)(4i\alpha)^2(2u-2i\alpha+2i\beta)^2(2u-2i\alpha-2i\beta)^2}\right.$$

$$+ \frac{2i\alpha}{(2u-2i\alpha)^2(4i\alpha)^2(2u-2i\alpha+2i\beta)^2(2u-2i\alpha-2i\beta)^2}$$

$$- \frac{4i\alpha}{(2u-2i\alpha)(4i\alpha)^3(2u-2i\alpha+2i\beta)^2(2u-2i\alpha-2i\beta)^2}$$

$$+ \frac{4i\alpha}{(2u-2i\alpha)(4i\alpha)^2(2u-2i\alpha+2i\beta)^3(2u-2i\alpha-2i\beta)^2}$$

$$+ \frac{4i\alpha}{(2u-2i\alpha)(4i\alpha)^2(2u-2i\alpha+2i\beta)^2(2u-2i\alpha-2i\beta)^3}$$

$$+ \frac{1}{(-2i\beta)(2u+2i\alpha+2i\beta)^2(2u+2i\beta-2i\alpha)^2(-4i\beta)^2}$$

$$+ \frac{2u+2i\beta}{(-2i\beta)^2(2u+2i\alpha+2i\beta)^2(2u+2i\beta-i\alpha)^2(-4i\beta)^2}$$

$$- \frac{4u+4i\beta}{(-2i\beta)(2u+2i\alpha+2i\beta)^3(2u+2i\beta-2i\alpha)^2(-4i\beta)^2}$$

$$- \frac{4u+4i\beta}{(-2i\beta)(2u+2i\alpha+2i\beta)^2(2u+2i\beta-2i\alpha)^3(-4i\beta)^2}$$

$$\left. + \frac{4u+4i\beta}{(-2i\beta)(2u+2i\alpha+2i\beta)^2(-4i\beta)^3(2u+2i\beta-2i\alpha)^2} \right\}.$$

In order to facilitate the integration over μ, we decomposed the expression within the brackets into a series of partial fractions. This is done in the following way.

If $\frac{\Phi(x)}{f(x)}$ is a proper rational fraction (the degree of the numerator is less than the degree of the denominator) and if $f(x) = (x-a)^{\alpha}(x-b)^{\beta} \ldots (x-m)^{\mu}$, then

$$\text{(B.5)} \quad \frac{\Phi(x)}{f(x)} = \frac{A_{\alpha}}{(x-a)^{\alpha}} + \frac{A_{\alpha-1}}{(x-a)^{\alpha-1}} + \ldots + \frac{A_1}{x-a}$$

$$+ \frac{B_{\beta}}{(x-b)^{\beta}} + \frac{B_{\beta-1}}{(x-b)^{\beta-1}} + \ldots + \frac{B_1}{x-b}$$

$$+ \quad \ldots \quad +$$

$$+ \frac{M_{\mu}}{(x-m)^{\mu}} + \frac{M_{\mu-1}}{(x-m)^{\mu-1}} + \ldots + \frac{M_1}{x-m}$$

where

$$A_{\alpha-k+1} = \frac{\psi_1^{(k-1)}(a)}{(k-1)!}, \quad B_{\beta-k+1} = \frac{\psi_2^{(k-1)}(b)}{(k-1)!}, \ldots,$$

$$M_{\mu-k+1} = \frac{\psi_m^{(k-1)}(m)}{(k-1)!},$$

and

$$\psi_1(x) = \frac{\Phi(x)(x-a)^{\alpha}}{f(x)}, \quad \psi_2(x) = \frac{\Phi(x)(x-b)^{\beta}}{f(x)}, \ldots,$$

$$\psi_m(x) = \frac{\Phi(x)(x-m)^{\mu}}{f(x)}.$$

For example, consider the first term in brackets in equation (B.4). This is

$$\frac{1}{(4i\alpha)^2 2^5 (u-i\alpha)(u-i\alpha+i\beta)^2 (u-i\alpha-i\beta)^2}$$

$$\psi_1(u) = \frac{1}{(4i\alpha)^2 2^5 (u-i\alpha+i\beta)^2 (u-i\alpha-i\beta)^2}$$

$$\psi_2(u) = \frac{1}{(4i\alpha)^2 2^5 (u-i\alpha)(u-i\alpha-i\beta)^2}$$

$$\psi_3(u) = \frac{1}{(4i\alpha)^2 2^5 (u-i\alpha)(u-i\alpha+i\beta)^2}$$

$$A_1 = \psi_1(i\alpha) = \frac{1}{(4i\alpha)^2 \; 2^5 \beta^4} = -\frac{1}{2^9 \alpha^2 \beta^4}$$

$$B_2 = \psi_2(i\alpha-i\beta) = \frac{1}{(4i\alpha)^2 \; 2^5 (-i\beta)(-2i\beta)^2} = \frac{1}{(4i\alpha)^2 2^7 i\beta^3} = \frac{i}{2^{11} \alpha^2 \beta^3}$$

$$B_1 = \psi_2'(i\alpha-i\beta) = -\frac{1}{(4i\alpha)^2 \; 2^6 \beta^4} = \frac{1}{2^{10} \alpha^2 \beta^4}$$

$$C_2 = \psi_3(i\alpha+i\beta) = \frac{1}{(4i\alpha)^2 2^7 i^3 \beta^3} = \frac{-i}{2^{11} \alpha^2 \beta^3}$$

$$C_1 = \psi_3'(i\alpha+i\beta) = \frac{-1}{(4i\alpha)^2 2^6 \beta^4} = \frac{1}{2^{10} \alpha^2 \beta^4}$$

This first term can then be written as

$$\frac{A_1}{u-i\alpha} + \frac{B_2}{(u-i\alpha+i\beta)^2} + \frac{B_1}{u-i\alpha+i\beta} + \frac{C_2}{(u-i\alpha+i\beta)^2} + \frac{C_1}{u-i\alpha-i\beta}$$

The integral over u becomes

(B.6)

$$\int_{-\infty}^{\infty} du \, \frac{2\pi^2 \epsilon^4 8m(\omega_1+\omega_2)u^3}{h^2\omega_1\omega_2} \, e^{\frac{i\omega_1\omega_2 \hbar u^2}{8m(\omega_1+\omega_2)}}$$

$$\cdot \left[\frac{A_2}{(u-i\alpha)^2} + \frac{A_1}{u-i\alpha} + \frac{B_2}{(u-i\alpha+i\beta)^2} + \frac{B_1}{u-i\alpha+i\beta} \right.$$

$$+ \frac{B_3}{(u-i\alpha+i\beta)^3} + \frac{C_2}{(u-i\alpha-i\beta)^2} + \frac{C_1}{u-i\alpha-i\beta} + \frac{C_3}{(u-i\alpha-i\beta)^3}$$

$$\left. + \frac{D_3}{(u+i\alpha+i\beta)^3} + \frac{D_2}{(u+i\alpha+i\beta)^2} + \frac{D_1}{u+i\alpha+i\beta} \right]$$

The contributions to the coefficients from the various terms are

term 1

$$A_1 = \frac{1}{(4i\alpha)^2 2^5 \beta^4} = \frac{-1}{2^9 \alpha^2 \beta^4} \qquad B_2 = \frac{1}{(4i\alpha)^2 2^7 i\beta^3} = \frac{i}{2^{11}\alpha^2\beta^3}$$

$$B_1 = \frac{-1}{(4i\alpha)^2 2^6 \beta^4} = \frac{1}{2^{10}\alpha^2\beta^4} \qquad C_2 = \frac{1}{(4i\alpha)^2 2^6 i^3 \beta^3} = \frac{-i}{2^{11}\alpha^2\beta^3}$$

$$C_1 = \frac{-1}{(4i\alpha)^2 2^6 \beta^4} = \frac{1}{2^{10}\alpha^2\beta^4}$$

term 2

$$A_2 = \frac{-i}{\alpha \; 2^9 \beta^4} \, , \quad A_1 = 0 \, , \quad B_2 = \frac{-i}{\alpha \; 2^{11} \beta^4} \, , \quad B_1 = \frac{-3}{\alpha \; \beta^5 2^{11}} \, ,$$

$$C_2 = \frac{-i}{\alpha \; 2^{11}\beta^4} \cdot C_1 = \frac{3}{\alpha \; 2^{11}\beta^5}$$

term 3

$$A_1 = \frac{1}{\alpha^2 2^9 \beta^4} \qquad B_2 = \frac{1}{\alpha^2 2^{11} i \beta^3} \qquad B_1 = \frac{-1}{\alpha^2 2^{10} \beta^4}$$

$$C_2 = \frac{i}{\alpha^2 2^{11} \beta^3} \qquad C_1 = \frac{-1}{\alpha^2 2^{10} \beta^4}$$

term 4

$$A_1 = \frac{-1}{\alpha\, 2^8 \beta^5} \qquad B_3 = \frac{-1}{\alpha\, 2^{10} \beta^3} \qquad B_2 = \frac{i}{\alpha\, 2^9\, \beta^4}$$

$$B_1 = \frac{1}{\alpha 2^9 \beta^5} + \frac{3}{\alpha 2^{12} \beta^5} = \frac{11}{\alpha 2^{12} \beta^5} \qquad C_2 = \frac{-i}{\alpha 2^{11} \beta^4} \qquad C_1 = \frac{5}{\alpha 2^{12} \beta^5}$$

term 5

$$A_1 = \frac{1}{\alpha\, 2^8\, \beta^5} \qquad B_2 = \frac{-i}{\alpha\, 2^{11} \beta^4} \qquad B_1 = \frac{-5}{\alpha\, 2^{12} \beta^5}$$

$$C_3 = \frac{1}{\alpha\, 2^{10} \beta^3} \qquad C_2 = \frac{i}{\alpha\, 2^9\, \beta^4}$$

$$C_1 = \frac{-1}{\alpha\, 2^9\, \beta^5} - \frac{3}{\alpha\, 2^{12} \beta^5} = \frac{-11}{\alpha\, 2^{12} \beta^5}$$

term 6

$$D_2 = \frac{i}{2^{11}\, \beta^3\, \alpha^2} \qquad D_1 = \frac{1}{2^{11}\, \beta^3\, \alpha^3}$$

$$B_2 = \frac{i}{2^{11}\, \beta^3\, \alpha^2} \qquad B_1 = \frac{1}{2^{11}\, \beta^3\, \alpha^3}$$

term 7

$$D_2 = \frac{i}{2^{11} \beta^4 \alpha} \qquad D_1 = 0 \qquad B_2 = \frac{-i}{2^{11} \beta^4 \alpha} \qquad B_1 = 0$$

term 8

$D_3 = \frac{-1}{2^{10}\beta^3\alpha}$ $\quad D_2 = 0$ $\quad D_1 = \frac{-1}{2^{10}\beta^3\alpha^3} + \frac{3}{2^{12}\beta^3\alpha^3} = \frac{-1}{2^{12}\beta^3\alpha^3}$

$B_2 = \frac{-i}{2^{11}\beta^3\alpha^2}$ $\quad B_1 = \frac{1}{2^{12}\beta^3\alpha^3}$

term 9

$D_2 = \frac{-i}{2^{11}\beta^3\alpha^2}$ $\quad D_1 = \frac{-1}{2^{12}\beta^3\alpha^3}$ $\quad B_3 = \frac{1}{2^{10}\beta^3\alpha}$

$B_2 = 0$ $\quad B_1 = \frac{1}{2^{10}\beta^3\alpha^3} - \frac{3}{2^{12}\beta^3\alpha^2} = \frac{1}{2^{12}\beta^3\alpha^3}$

term 10

$D_2 = \frac{i}{2^{11}\beta^4\alpha}$ $\quad D_1 = 0$ $\quad B_2 = \frac{-i}{2^{11}\beta^4\alpha}$ $\quad B_1 = 0$

Collecting the contributions to the coefficients from the various terms we have

$A_1 = 0$ $\quad A_2 = \frac{-i}{\alpha\ 2^9\beta^4}$

$B_3 = 0$ $\quad B_2 = 0$ $\quad B_1 = 0$

$C_1 = 0$ $\quad C_3 = \frac{1}{\alpha\ 2^{10}\beta^3}$ $\quad C_2 = \frac{i}{\alpha\ 2^{10}\beta^4}$

$D_3 = \frac{-1}{2^{10}\beta^3\alpha}$ $\quad D_2 = \frac{i}{2^{10}\beta^4\alpha}$ $\quad D_1 = 0$

Note that

$$C_2 = D_2 \qquad C_3 = -D_3 \qquad A_2 = -2C_2$$

and all the rest are zero.

Carrying out the integrations indicated in equation (B.6), denoting $\frac{\omega_1\omega_2}{\omega_1+\omega_2}$ by x, and using the values of the coefficients just derived, we get:

$$(B.7)\quad \frac{\alpha\ \beta\ 2\pi^3 4^4 8m}{\hbar^2 x}\Bigg\{-\frac{i\ A_2\hbar^2 x\pi\alpha}{4m}\, e^{-\frac{ix\hbar^2\alpha^2}{8m}}\left(1-\Phi\left(\alpha\hbar\sqrt{\frac{-ix}{8m}}\right)\right)$$

$$-\frac{2C_2 i\hbar^2 x\ (\alpha+\beta)}{4m}\, e^{-\frac{ix\hbar^2(\alpha+\beta)^2}{8m}}\left(1-\Phi\left(\hbar(\alpha+\beta)\sqrt{\frac{-ix}{8m}}\right)\right)$$

$$-\frac{2iC_3(\alpha+\beta)\hbar^4x^2}{32m^2}\Bigg[\frac{\sqrt{\pi}}{\hbar\sqrt{\frac{-ix}{8m}}}-\pi(\alpha+\beta)e^{-\frac{ix\hbar^2(\alpha+\beta)^2}{8m}}\Big(1-\Phi\Big(\hbar(\alpha+\beta)$$

$$\cdot\sqrt{\frac{-ix}{8m}}\Big)\Big)\Bigg]\Bigg\}$$

where Φ is the error function:

$$\Phi(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt\ .$$

We should notice here the relatively simple form of the expression, considering the messy looking expression (B.4) before the integration over u was done.

APPENDIX C

A Small Electric Charge in an Infinite Electron Gas Treated by Perturbation Theory

$$(C.1)\ \bar{V}(r',r'',\omega) = \frac{2\pi}{ih}\Big[\sum_{k'}^{\text{unocc}}\sum_{k''}^{\text{occ}} u_k(r')\,\bar{u}_{k'}(r'')\,u_{k''}(r'')\,\bar{u}_{k''}(r')$$

$$\cdot\ \delta_-\Big(\frac{E_{k'}-E_{k''}}{h}+\omega\Big)$$

$$+\sum_{k'}^{\text{occ}}\sum_{k''}^{\text{unocc}} u_{k'}(r')\bar{u}_{k'}(r'')u_{k''}(r'')\bar{u}_{k''}(r')\ \delta_+\Big(\frac{E_{k'}-E_{k''}}{h}+\omega\Big)\Big]$$

Say the u(r) are bound hydrogenic wave functions for the first N levels. Beyond that they become continuum functions where we use plane waves for the continuum.

$$\delta_{\pm}(x) = \mp\frac{1}{2\pi i}\frac{P}{x}+\frac{1}{2}\delta(x)$$

where P means principal value.

Then the first term of c_1 will be of the form

$$(C.2)\ \frac{2\pi}{ih}\Big[\sum_{k'}^{\text{unocc}}\sum_{k''}^{N} e^{ik'\cdot r'}\,e^{-ik'\cdot r''}\,u_{k''}(r'')\,\bar{u}_{k''}(r')\,\delta_-\Big(\frac{E_{k'}-E_{k''}}{h}+\omega\Big)$$

$$-\sum_{k'}^{\text{unocc}}\sum_{k''=N}^{k''_F} e^{ik'\cdot(r'-r'')}\,e^{ik''\cdot(r''-r')}\,\delta_-\Big(\frac{E_{k'}-E_{k''}}{h}+\omega\Big)\Big]$$

Second term

$$(C.3)\ \frac{2\pi}{ih}\Big[\sum_{k'}^{N}\sum_{k''}^{\text{unocc}} u_{k'}(r')\,\bar{u}_{k'}(r'')\,e^{ik''\cdot r''}\,u^{-ik''\cdot r'}\,\delta_+\Big(\frac{E_{k'}-E_{k''}}{h}+\omega\Big)$$

$$+\sum_{k'=N}^{k'_F}\sum_{k''}^{\text{unocc}} e^{ik'\cdot(r'-r'')}\,e^{ik''\cdot(r''-r')}\,\delta_+\Big(\frac{E_{k'}-E_{k''}}{h}+\omega\Big)$$

Now we want $V^*(r',r,\omega) = \int \overline{V}(r',r'',\omega) \dfrac{1}{|r''-r|} dr''$

If $\overline{V}(r',r'') \equiv \overline{V}(r'-r'')$, then

$$\overline{V}(r'-r'',\omega) = \int \overline{V}(k,\omega)\, e^{ik\cdot(r'-r'')}\, d^3k$$

and

$$\begin{aligned} V^*(r',r) &= \iint \overline{V}(k,\omega)\, e^{ik(r'-r'')}\, d^3k\; v(k')e^{ik'\cdot(r''-r)} d^3k' d^3r'' \\ &= \iint \overline{V}(k,\omega)e^{ik\cdot r'} v(k')e^{-ik'r}\, \delta(k-k')\, d^3k\, d^3k' \\ &= \int \overline{V}(k,\omega)\, e^{ik\cdot(r'-r)}\, v(k)\, d^3k\, . \end{aligned}$$

Let $\overline{V}(r',r'',\omega) = \overline{V}_I + \overline{V}_{II}$.

V_{II} contains just plane waves; V_I contains the Coulomb functions.

$$\begin{aligned} V^*(r,r',\omega) &= \int \overline{V}_I(r',r'',\omega) \frac{1}{|r''-r|} d^3r'' + \int \overline{V}_{II}(k,\omega)e^{ik\cdot(r'-r)} \cdot v(k)\, d^3k \\ &= V_I^* + V_{II}^* \, . \end{aligned}$$

V_{II}^* is the same as the homogeneous case.

We make the simplification that there is only one bound state -- the ground state:

$$u_0 = 2\left(\frac{z}{a_0}\right)^{3/2} e^{-zr''/a_0}$$

to evaluate V_I^*. Then, the first term of (C.2) is

$$(C.4)\ \frac{2\pi}{ih} \int \sum_{k'}^{\text{unocc}} e^{ik'\cdot r'}\, e^{-ik'\cdot r''}\, u_0(r'')\, \bar{u}_0(r')\, \delta_-\left(\frac{E_{k'}-E_0}{h}+\omega\right)\frac{1}{|r''-r|}\, d^3r''$$

The first term of (C.3) is

$$(C.5)\ \frac{2\pi}{ih} \int \sum_{k''}^{\text{unocc}} u_0(r')\bar{u}_0(r'')e^{ik''\cdot r''}e^{-ik''\cdot r'}\ \delta_+\left(\frac{E_0-E_{k''}}{\hbar}+\omega\right)\frac{1}{|r''-r|}\, d^3r''$$

We must integrate

$$\int e^{-ik'\cdot r''}\, u_0(r'')\, \frac{1}{|r''-r|}\, dr''$$

and

$$\int e^{ik''\cdot r''}\, u_0(r'')\, \frac{1}{|r''-r|}\, dr'' .$$

Now

$$\frac{1}{|r''-r|} = 4\pi \sum_{\ell'=0}^{\infty} \sum_{m=-\ell'}^{\ell'} \frac{1}{2\ell'+1}\, \frac{r_<^{\ell'}}{r_>^{\ell'+1}}\, Y^*_{\ell' m}(\theta'',\phi'')Y_{\ell' m}(\theta,\phi)$$

$$e^{-ik'r''\cos\theta''} = \sum_{\ell=0}^{\infty} (2\ell+1)(-i)^{\ell}\, j_{\ell}(k'r'')\, P_{\ell}(\cos\theta'')$$

$$e^{ik''r''\cos\theta''} = \sum_{\ell=0}^{\infty} (2\ell+1)(i)^{\ell}\, j_{\ell}(k''r'')\, P_{\ell}(\cos\theta'')$$

and

$$P_{\ell} = Y_{\ell}\sqrt{\frac{4\pi}{2\ell+1}} .$$

Consider the integral

$$(C.6)\quad \int e^{-ik'r''\cos\theta''}\left(\frac{z}{a_0}\right)^{3/2} 2e^{-zr''/a_0}\frac{1}{|r''-r|}\, 2\pi\, d\cos\theta'' r''^2 dr''$$

From the angular part we get a factor of $\sqrt{\frac{4\pi}{2\ell+1}}\,\delta(\ell'-\ell)\delta(m-0)$

So (C.6) becomes

$$(C.7)\quad \sum_{\ell=0}^{\infty} 2\sqrt{\frac{4\pi}{2\ell+1}}\,\frac{4\pi}{2\ell+1}(2\ell+1)(-i)^{\ell}\left(\frac{z}{a_0}\right)^{3/2}$$

$$\cdot\left[\int_0^r j_\ell(k'r'')\frac{r''^{\ell}}{r^{\ell+1}}e^{-zr''/a_0}r''^2\,dr''\right.$$

$$\left.+\int_r^{\infty} j_\ell(k'r'')\frac{r^{\ell}}{r''^{\ell+1}}e^{-zr''/a_0}r''^2\,dr''\right]Y_{\ell 0}(\theta,\phi)\ .$$

For the time being we will just consider the $\ell = 0$ term to see how the problem develops. Then we have

$$2(4\pi)^{3/2}\left(\frac{z}{a_0}\right)^{3/2}\left[\int_0^r j_0(k'r'')\frac{r''^0}{r^1}e^{-zr''/a_0}r''^2\,dr''\right.$$

$$\left.+\int_r^{\infty} j_0(k'r'')\frac{r^0}{r''^1}e^{-zr''/a_0}r''^2\,dr''\right]\ .$$

Using $j_0(kr) = \sin kr\ /\ kr$ and integrating by parts we get

$$(C.8)\quad 2(4\pi)^{3/2}\left(\frac{z}{a_0}\right)^{3/2}\left[\ \frac{1}{r}\left\{\frac{r}{k'}e^{-zr/a_0}\left\{\frac{\frac{-z}{a_0}\sin k'r-k'\cos k'r}{\left(\frac{z^2}{a_0^2}+k'^2\right)}\right\}\right.\right.$$

$$+\frac{z}{a_0k'}\,\frac{e^{-zr/a_0}}{\left[\frac{z^2}{a_0^2}+k'^2\right]^2}\left[-\frac{z}{a_0}\sin k'r-k'\cos kr\right]+$$

$$+ \frac{e^{-zr/a_0}}{[\frac{z^2}{a_0^2} + k'^2]^2} [- \frac{z}{a_0} \cos k'r + k' \sin k'r]$$

$$+ \frac{2z}{a_0} \frac{1}{[\frac{z^2}{a_0^2} + k'^2]^2} \Big\}]$$

$$+ \frac{2(4\pi)^{3/2} (\frac{z}{a_0})^{3/2}}{k'[\frac{z^2}{a_0} + k'^2]} e^{-zr/a_0} (z/a_0 \sin k'r + k' \cos k'r)$$

Denote all this by $F(k',r)e^{-zr/a_0}$. So,

$$\text{(C.9)} \quad V_I^*(r',r) = \frac{2\pi}{i\hbar} \sum_{k'}^{\text{unocc}} e^{ik'\cdot r'} \bar{u}_0(r') F(k'r) e^{-zr/a_0} \delta_-(\frac{E_{k'} - E_0}{\hbar} + \omega)$$

$$+ \frac{2\pi}{i\hbar} \sum_{k''}^{\text{unocc}} u_0(r') F(k''r) e^{-zr/a_0} e^{-ik''\cdot r'} \delta_+(\frac{E_0 - E_{k''}}{\hbar} + \omega)$$

$$\mu_i(\omega) = \int \chi(r') V^*(r',r,\omega) \phi(r) d^3r\, d^3r' .$$

Try

$$\chi(r') = e^{-ik\cdot r'} , \qquad \phi(r) = e^{+ik\cdot r} .$$

Interchanging the sum and integral,

$$\text{(C.10)} \quad \mu_i(\omega) = \frac{2\pi}{i\hbar} \sum_{k'}^{\text{unocc}} (\int e^{i(k'-k)\cdot r'} u_0(r') d^3r')$$

$$\cdot \int F(k'r) e^{-zr/a_0} e^{ik\cdot r} d^3r] \delta_-(\frac{E_{k'} - E_0}{\hbar} + \omega)$$

$$+ \frac{2\pi}{i\hbar} \sum_{k''} \int u_0(r') e^{-i(k+k'')\cdot r'} d^3r' .$$

$$\cdot \int F(k''r)\, e^{-zr/a_0}\, e^{ik\cdot r}\, d^3r]\ \delta_+[\frac{E_0-E_{k''}}{\hbar} + \omega]$$

Consider the integral over r'.

$$2(\frac{z}{a_0})^{3/2} \int e^{-zr'/a_0}\, e^{-i(k'-k)\cdot r'}\, d^3r'$$

$$= \int e^{i(k'-k)\cdot r'}\, u_0(r')\, d^3r'.$$

Ths integral when evaluated is

$$\text{(C.11)} \qquad 4\pi(\frac{z}{a_0})^{3/2}\ \frac{4}{[\frac{z^2}{a_0^2} - (k'-k)^2 + 4(k'-k)^2]}$$

and

$$\text{(C.12)} \quad \int u_0(r')\, e^{-i(k+k'')\cdot r''}\, d^3r'$$

$$= 4\pi(\frac{z}{a_0})^{3/2}\ \frac{4}{[\frac{z^2}{a_0^2} - (k+k'')^2]^2 + 4(k+k'')^2}$$

To estimate the order of magnitude of this term we note that

$$k'_{min} = k_F \sim 10^{\infty} \sim \frac{z}{a_0}$$

and

$$k' >> k .$$

Therefore, this term is of the order

$$\sim \frac{(\frac{z}{a_0})^{3/2}}{k'^4} \sim \frac{(k')^{3/2}}{k'^4} \sim k'^{-5/2}$$

and the term is a maximum for $k' = k_F$. So, the maximum value is about $k_F^{-5/2}$. Consider

$$\int F(k'r)\, e^{-zr/a_0}\, e^{ik\cdot r}\, d^3r$$

$a_0 \sim 10^{-\infty}$ and $F(k'r)$ is sinusoidal.

Therefore the integrand must be very small unless

$$r \text{ is small}, \quad r \lesssim 10^{-8}$$

Also, judging from results for the homogeneous gas, it seems reasonable to assume k small, i.e. $k/k_F \ll 1$. Therefore

$$e^{ik\cdot r} \sim 1 .$$

This would justify considering only the $\ell = 0$ case. The minimum value of k' is $k_{Fermi} \sim 10^8$. Also $z/a_0 \sim 10^8$. We note that the first and last terms in $F(k'r)$ cancel.

$$\text{(C.13)} \quad F(k'r) = 2(4\pi)^{3/2}\left(\frac{z}{a_0}\right)^{3/2} \frac{1}{\left[\frac{z^2}{a_0^2} + k'^2\right]^2} \frac{1}{r}$$

$$\cdot\left[- \frac{z_0^2}{a_0^2 k'} \sin k'r - \frac{z}{a_0} \cos k'r - \frac{z}{a_0} \cos k'r + k' \sin k'r + \frac{2z}{a_0}\right]$$

$$= \frac{2(4\pi)^{3/2}\left(\frac{z}{a_0}\right)^{3/2}}{\left[\frac{z^2}{a_0^2} + k'^2\right]^2} \frac{1}{r} \left[\sin k'r\left[k' - \frac{z_0^2}{a_0^2 k'}\right] - \frac{2z}{a_0} \cos k'r + \frac{2z}{a_0}\right].$$

Evaluating $\int_0^\infty F(k'r)\, e^{-zr/a_0}\, 4\pi\, r^2\, dr$, we have:

$$(C.14)\quad \frac{2(4\pi)^{3/2}(\frac{z}{a_0})^{3/2}}{[\frac{z^2}{a_0^2}+k'^2]^2}\left\{\left[4\pi\,\frac{z}{a_0}(k'^2-\frac{z_0^2}{a_0^2}+\frac{z}{a_0}\,k'+\frac{z_0^3}{a_0^3k'})\right.\right.$$

$$\left.\left.-\,8\pi\,\frac{z}{a_0}[\,\frac{z^2}{a_0^2}-k'^2]\right]\Big/\,[\,\frac{z^2}{a_0^2}+k'^2]^2\;+\;\frac{8\pi}{z/a_0}\right\}$$

$\int_0^\infty F(k''r)\,e^{-zr/a_0}\,4\pi\,r^2\,dr$ is the same with k' replaced by k''.

Now we have to sum over k' and k'' with both k' and k'' going from k_F to ∞, and $k_F \sim 10^8$ for a high density gas. We will therefore approximate (C.14) in order to get an estimate of the magnitude.

The expression in the brackets is $\sim 1/k'$ for k' very large. (The maximum of the expression is for $k' = k_F \cong z/a_0$. Therefore

$$\int_0^\infty F(k'r)\,e^{-zr/a_0}\,4\pi\,r^2\,dr \sim \frac{(\frac{z}{a_0})^{3/2}}{k'^4\;k'} \sim \frac{k'^{3/2}}{k'^5} = k_F'^{-7/2}$$

$$\cong \text{ maximum value.}$$

The magnitude of the perturbation term is

$$\sum_{k'=k_F}^{\infty} k'^{-5/2}\cdot k'^{-7/2} = \sum_{k'=k_F}^{\infty} k'^{-6}$$

and the maximum value is $(10^{-8})^6 = 10^{-48}$.

Therefore for z positive there is no measurable effect. The inclusion of additional terms would only give more terms of this order of magnitude.

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